



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2017 – 01:38 AM EDT

PDB ID : 5V2C
Title : RE-REFINEMENT OF CRYSTAL STRUCTURE OF PHOTOSYSTEM II COMPLEX
Authors : Wang, J.; Wiwczar, J.M.; Brudvig, G.W.
Deposited on : unknown
Resolution : 1.90 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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

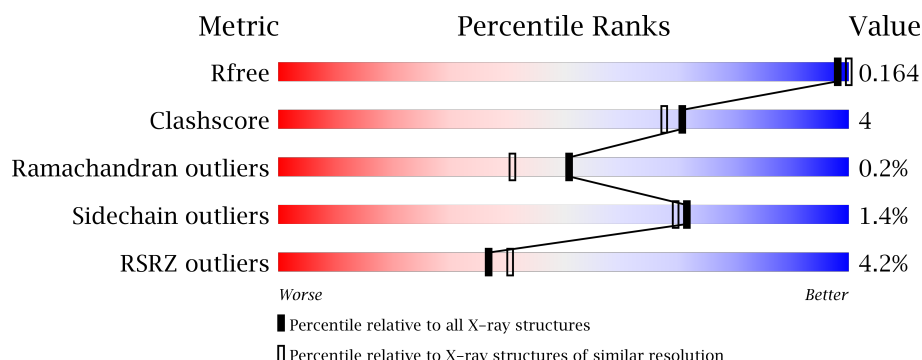
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>0.1%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	a	344	<div> <div>0.1%</div> <div>96%</div> <div>.</div> <div>.</div> </div>
2	B	506	<div> <div>4%</div> <div>90%</div> <div>9%</div> </div>
2	b	506	<div> <div>6%</div> <div>96%</div> <div>.</div> </div>
3	C	458	<div> <div>0.1%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>

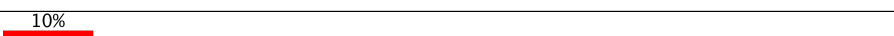
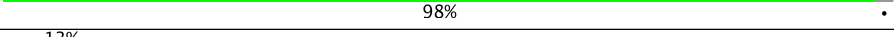
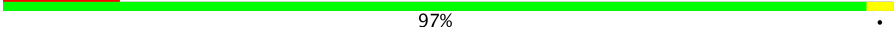
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Mol	Chain	Length	Quality of chain
3	c	458	
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	245	
13	o	245	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	BCT	m	104[A]	-	-	-	X
23	BCT	m	104[B]	-	-	-	X
24	CLA	A	606	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	609	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	a	410	X	-	-	-
24	CLA	b	602	X	-	-	X
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
27	PL9	A	611	-	-	-	X
27	PL9	a	412	-	-	-	X
28	SQD	A	616	-	-	-	X
28	SQD	A	622	-	-	-	X
28	SQD	F	104	-	-	-	X
28	SQD	a	417	-	-	-	X
28	SQD	h	105	-	-	-	X
28	SQD	l	102	-	-	-	X
29	LMG	A	613	-	-	-	X
29	LMG	B	634	-	-	-	X
29	LMG	C	520	-	-	-	X
29	LMG	C	526	-	-	-	X
29	LMG	a	414	-	-	-	X
29	LMG	b	621	-	-	-	X
29	LMG	d	412	-	-	-	X
29	LMG	z	101	-	-	-	X
30	GOL	A	615	-	-	-	X
30	GOL	B	625	-	-	-	X
30	GOL	B	635	-	-	-	X
30	GOL	C	523	-	-	-	X
30	GOL	C	528	-	-	X	X
30	GOL	D	402	-	-	-	X
30	GOL	D	413	-	-	-	X
30	GOL	O	304	-	-	-	X
30	GOL	O	305	-	-	-	X
30	GOL	O	306	-	-	-	X
30	GOL	U	201	-	-	-	X
30	GOL	V	206	-	-	-	X
30	GOL	a	416	-	-	-	X
30	GOL	b	629	-	-	-	X
30	GOL	c	525	-	-	-	X
30	GOL	c	528	-	-	-	X
30	GOL	c	529	-	-	-	X
30	GOL	d	402	-	-	-	X
30	GOL	t	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	GOL	u	202	-	-	-	X
30	GOL	v	203	-	-	-	X
30	GOL	v	207	-	-	-	X
31	LMT	A	617	-	-	-	X
31	LMT	F	102	-	-	-	X
31	LMT	J	103	-	-	-	X
31	LMT	M	102	-	-	-	X
31	LMT	a	401	-	-	-	X
31	LMT	c	521	-	-	-	X
31	LMT	f	101	-	-	-	X
31	LMT	j	103	-	-	-	X
31	LMT	m	101	-	-	-	X
31	LMT	t	103	-	-	-	X
31	LMT	u	203	-	-	-	X
32	LHG	A	618	-	-	-	X
32	LHG	D	411	-	-	-	X
32	LHG	a	419	-	-	-	X
33	PG4	A	619	-	-	-	X
33	PG4	B	637	-	-	-	X
33	PG4	B	639	-	-	-	X
33	PG4	B	642	-	-	-	X
33	PG4	C	535	-	-	-	X
33	PG4	C	536	-	-	-	X
33	PG4	E	102	-	-	-	X
33	PG4	H	107	-	-	-	X
33	PG4	I	102	-	-	-	X
33	PG4	J	104	-	-	-	X
33	PG4	J	105	-	-	-	X
33	PG4	K	102	-	-	-	X
33	PG4	U	202	-	-	-	X
33	PG4	V	209	-	-	-	X
33	PG4	V	210	-	-	-	X
33	PG4	V	211	-	-	-	X
33	PG4	X	101	-	-	-	X
33	PG4	X	102	-	-	-	X
33	PG4	a	421	-	-	-	X
33	PG4	b	636	-	-	-	X
33	PG4	c	532	-	-	-	X
33	PG4	c	533	-	-	-	X
33	PG4	c	534	-	-	-	X
33	PG4	e	104	-	-	-	X
33	PG4	i	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	PG4	j	104	-	-	-	X
33	PG4	x	102	-	-	-	X
34	PGE	B	645	-	-	-	X
34	PGE	B	648	-	-	-	X
34	PGE	B	649	-	-	-	X
34	PGE	C	539	-	-	-	X
34	PGE	C	540	-	-	-	X
34	PGE	E	104	-	-	-	X
34	PGE	E	109	-	-	-	X
34	PGE	O	308	-	-	-	X
34	PGE	O	309	-	-	-	X
34	PGE	T	104	-	-	-	X
34	PGE	V	214	-	-	-	X
34	PGE	V	215	-	-	-	X
34	PGE	b	638	-	-	-	X
34	PGE	b	643	-	-	-	X
34	PGE	c	539	-	-	-	X
34	PGE	c	540	-	-	-	X
34	PGE	i	105	-	-	-	X
34	PGE	o	306	-	-	-	X
34	PGE	o	309	-	-	-	X
34	PGE	t	105	-	-	-	X
35	P6G	A	623	-	-	-	X
35	P6G	A	624	-	-	-	X
35	P6G	B	652	-	-	-	X
35	P6G	D	417	-	-	-	X
35	P6G	E	110	-	-	-	X
35	P6G	T	105	-	-	-	X
35	P6G	d	415	-	-	-	X
35	P6G	d	416	-	-	-	X
35	P6G	j	106	-	-	-	X
36	EDO	B	656	-	-	-	X
36	EDO	E	112	-	-	-	X
36	EDO	O	311	-	-	-	X
36	EDO	X	104	-	-	-	X
38	HTG	C	522	-	-	-	X
38	HTG	C	529	-	-	-	X
38	HTG	H	101	-	-	-	X
38	HTG	V	204	-	-	-	X
38	HTG	a	418	-	-	-	X
38	HTG	c	523	-	-	-	X
38	HTG	c	531	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	HTG	h	101	-	-	-	X
39	1PE	B	654	-	-	-	X
39	1PE	V	217	-	-	-	X
39	1PE	e	105	-	-	-	X
40	DGD	C	518	-	-	-	X
40	DGD	D	408	-	-	-	X
40	DGD	d	408	-	-	-	X
43	2PE	V	216	-	-	-	X

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 57584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2639	1730	434	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2639	1730	434	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	11	0
			4032	2646	671	702	13			
2	b	506	Total	C	N	O	S	0	10	0
			4037	2649	670	705	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	SER	-	expression tag	UNP D0VWR1
B	507	ASP	-	expression tag	UNP D0VWR1
b	506	SER	-	expression tag	UNP D0VWR1
b	507	ASP	-	expression tag	UNP D0VWR1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3508	2297	585	613	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	c	458	Total	C	N	O	S	0	4	0
			3553	2324	592	624	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	GLU	-	expression tag	UNP D0VWR7
C	17	ALA	-	expression tag	UNP D0VWR7
C	18	ALA	-	expression tag	UNP D0VWR7
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	16	GLU	-	expression tag	UNP D0VWR7
c	17	ALA	-	expression tag	UNP D0VWR7
c	18	ALA	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2731	1810	445	464	12			
4	d	342	Total	C	N	O	S	0	2	0
			2741	1815	448	466	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	3	0
			676	441	110	125				
5	e	81	Total	C	N	O		0	2	0
			668	436	107	125				

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	39	Total	C	N	O	S	0	2	0
			294	197	46	50	1			
9	j	39	Total	C	N	O	S	0	0	0
			281	187	43	50	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	2	GLU	MET	conflict	UNP Q7DGD4
j	2	GLU	MET	conflict	UNP Q7DGD4

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	2	0
			315	211	49	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	2	0
			286	190	42	53	1			
12	m	35	Total	C	N	O	S	0	2	0
			289	193	42	52	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	245	Total	C	N	O	S	0	6	0
			1904	1192	317	391	4			
13	o	245	Total	C	N	O	S	0	5	0
			1902	1189	320	389	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	2	ALA	-	expression tag	UNP D0VWR2
O	3	ALA	-	expression tag	UNP D0VWR2
o	2	ALA	-	expression tag	UNP D0VWR2
o	3	ALA	-	expression tag	UNP D0VWR2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	2	0
			271	190	36	42	3			
14	t	30	Total	C	N	O	S	0	2	0
			271	190	36	42	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	2	0
			786	499	130	157				
15	u	97	Total	C	N	O		0	0	0
			774	491	129	154				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1077	683	181	209	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	1	0
			219	145	37	34	3			
17	y	29	Total	C	N	O	S	0	1	0
			220	146	37	33	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	S	0	1	0
			300	201	47	51	1			
18	x	40	Total	C	N	O	S	0	0	0
			295	196	47	51	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	initiating methionine	UNP D0VWR4

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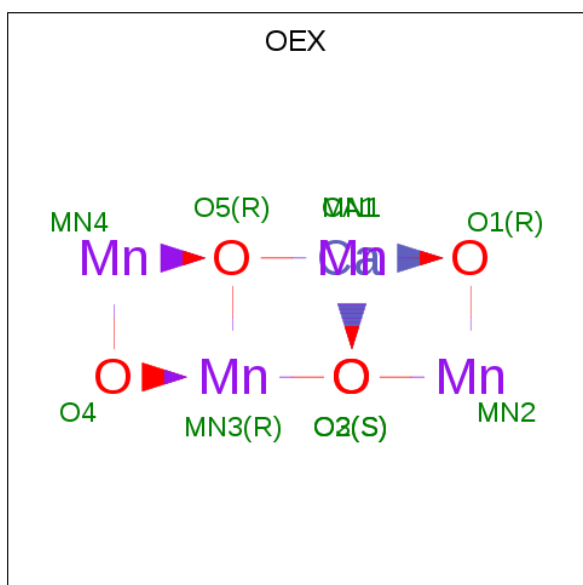
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Chain	Residue	Modelled	Actual	Comment	Reference
x	1	MET	-	initiating methionine	UNP D0VWR4

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

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

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

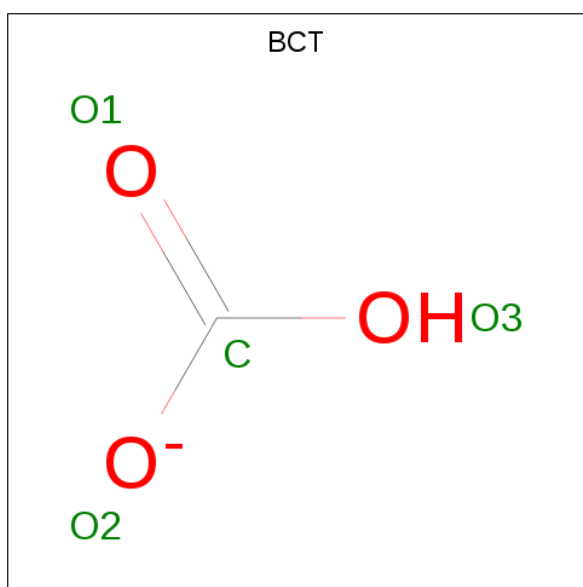
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

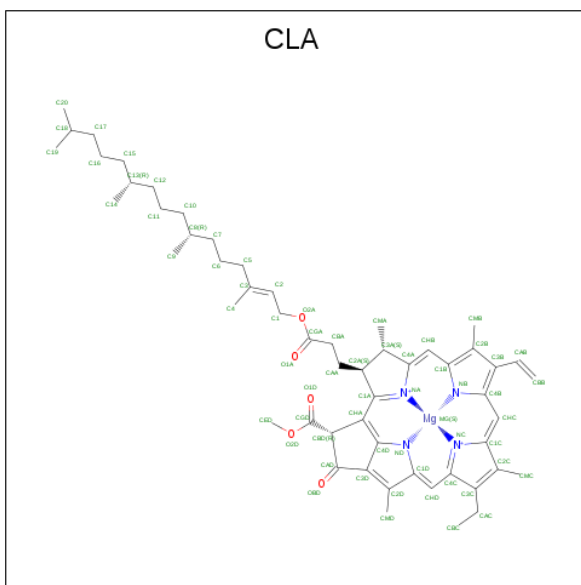
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	0
			2	2		
22	A	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		
22	V	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			4	1	3		
23	a	1	Total	C	O	0	0
			4	1	3		
23	m	1	Total	C	O	0	1
			8	2	6		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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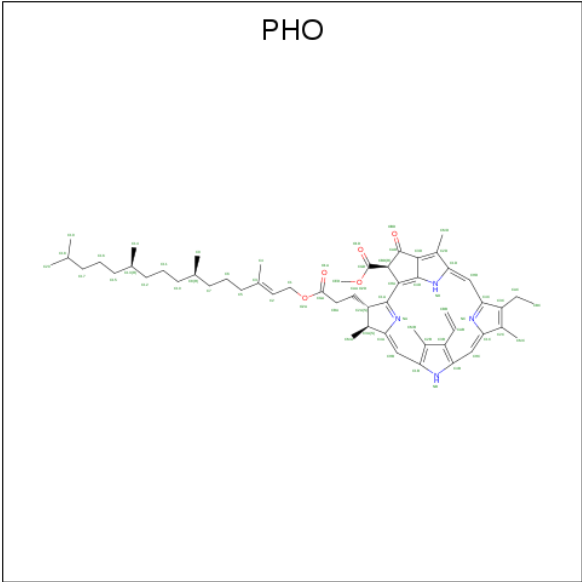
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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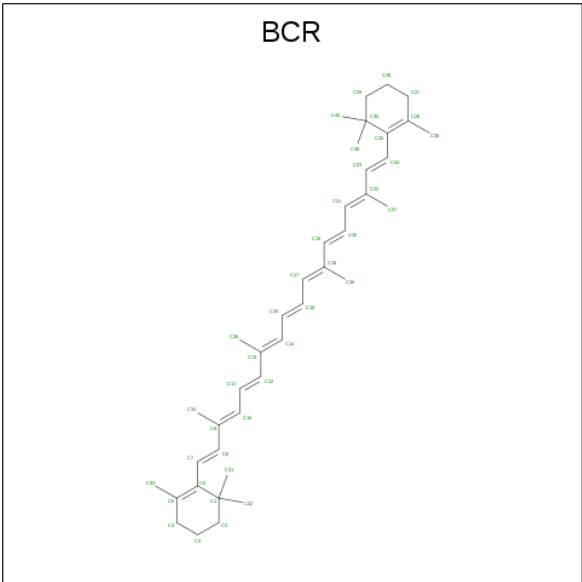
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



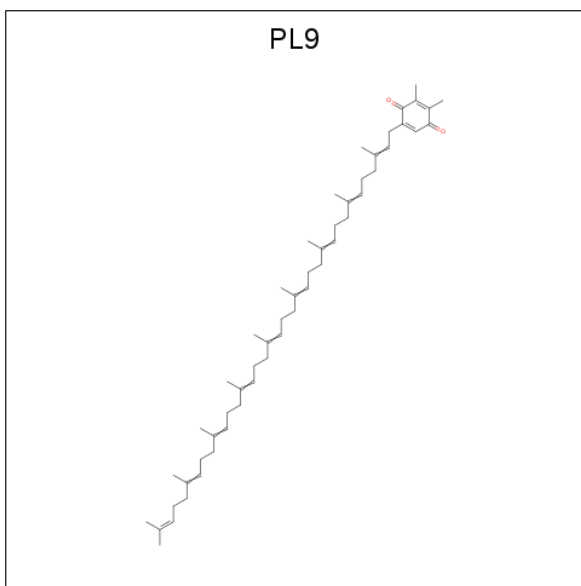
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



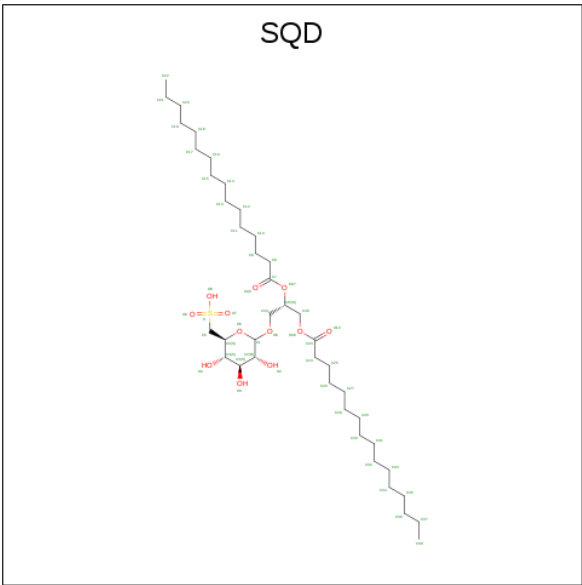
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0

- Molecule 27 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: $C_{53}H_{80}O_2$).



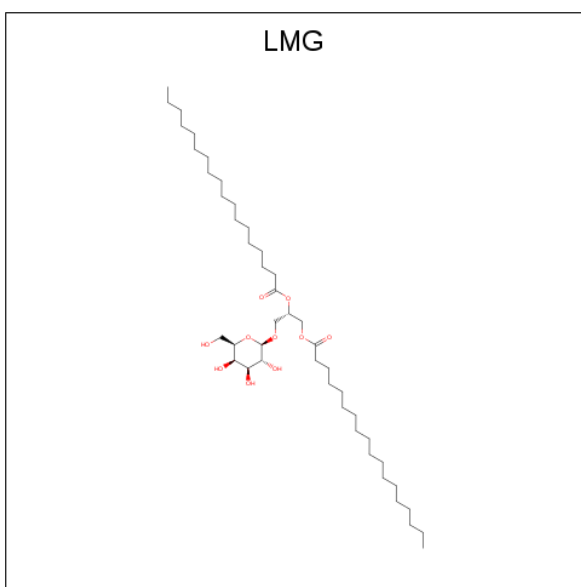
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



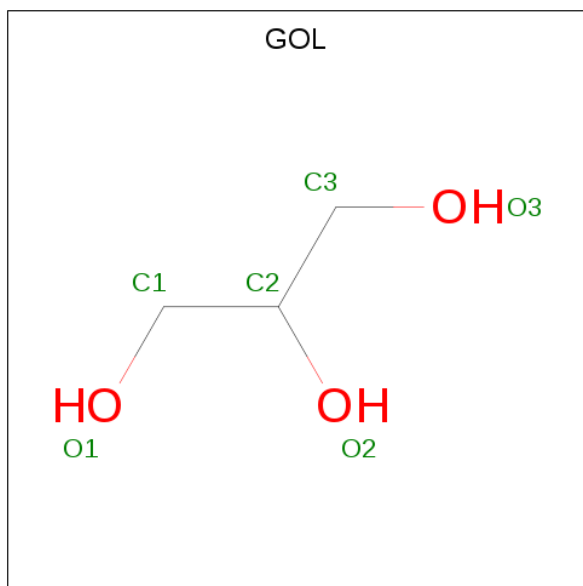
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	F	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	0
			54	41	12	1		
28	h	1	Total	C	O	S	0	0
			54	41	12	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		
28	x	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total 51	C 41	O 10	0	0
29	B	1	Total 51	C 41	O 10	0	0
29	B	1	Total 55	C 45	O 10	0	0
29	C	1	Total 51	C 41	O 10	0	0
29	C	1	Total 51	C 41	O 10	0	0
29	C	1	Total 55	C 45	O 10	0	0
29	J	1	Total 47	C 37	O 10	0	0
29	a	1	Total 51	C 41	O 10	0	0
29	b	1	Total 51	C 41	O 10	0	0
29	c	1	Total 51	C 41	O 10	0	0
29	c	1	Total 51	C 41	O 10	0	0
29	d	1	Total 55	C 45	O 10	0	0
29	j	1	Total 47	C 37	O 10	0	0
29	z	1	Total 55	C 45	O 10	0	0

- Molecule 30 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	D	1	Total 6	C 3	O 3	0	0
30	D	1	Total 6	C 3	O 3	0	0
30	D	1	Total 6	C 3	O 3	0	0
30	F	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	T	1	Total 6	C 3	O 3	0	0
30	T	1	Total 6	C 3	O 3	0	0
30	U	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	a	1	Total 6	C 3	O 3	0	0
30	a	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0

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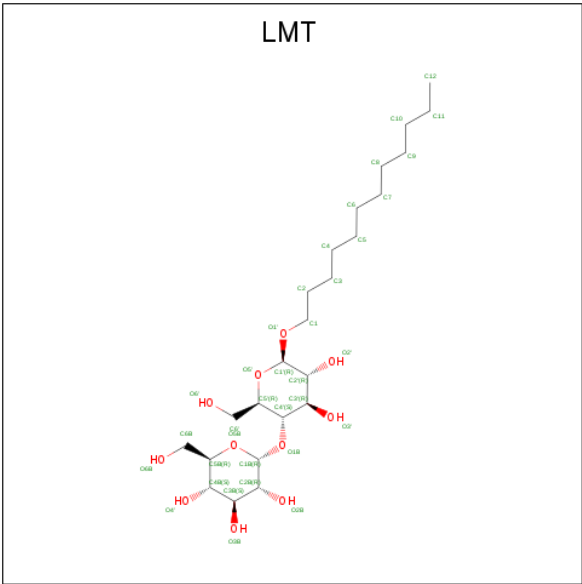
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	e	1	Total	C	O	0	0
			6	3	3		
30	f	1	Total	C	O	0	0
			6	3	3		
30	f	1	Total	C	O	0	0
			6	3	3		
30	m	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	t	1	Total	C	O	0	0
			6	3	3		
30	u	1	Total	C	O	0	0
			6	3	3		
30	u	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	y	1	Total	C	O	0	0
			6	3	3		

- Molecule 31 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



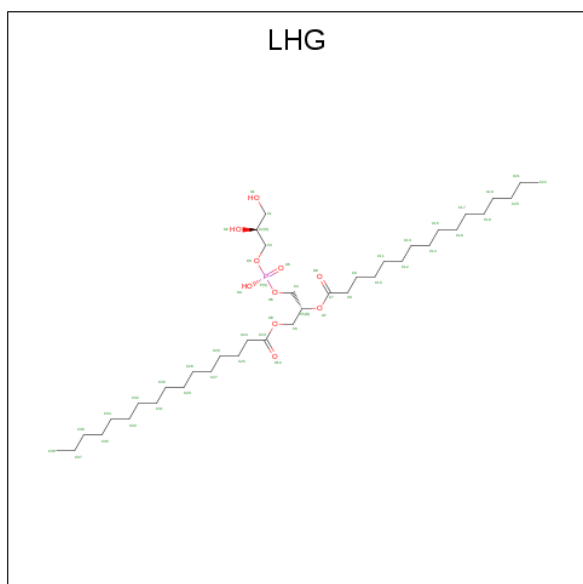
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	C	1	Total	C	O	0	0
			35	24	11		
31	F	1	Total	C	O	0	0
			35	24	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	J	1	Total	C	O	0	0
			35	24	11		

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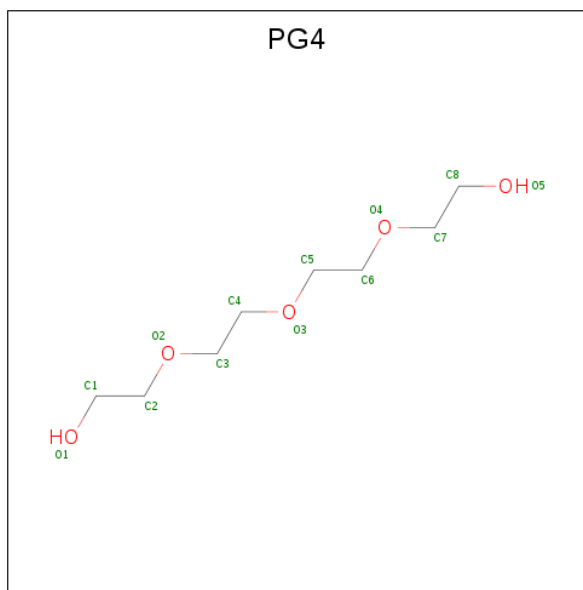
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	Y	1	Total	C	O	0	0
			35	24	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			35	24	11		
31	c	1	Total	C	O	0	0
			35	24	11		
31	f	1	Total	C	O	0	0
			35	24	11		
31	j	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	t	1	Total	C	O	0	0
			35	24	11		
31	u	1	Total	C	O	0	0
			35	24	11		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	0
			42	31	10	1		
32	B	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			42	31	10	1		
32	a	1	Total	C	O	P	0	0
			41	30	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	e	1	Total	C	O	P	0	0
			42	31	10	1		
32	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 33 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	D	1	Total	C	O	0	0
			13	8	5		
33	E	1	Total	C	O	0	0
			13	8	5		
33	E	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	I	1	Total	C	O	0	0
			13	8	5		

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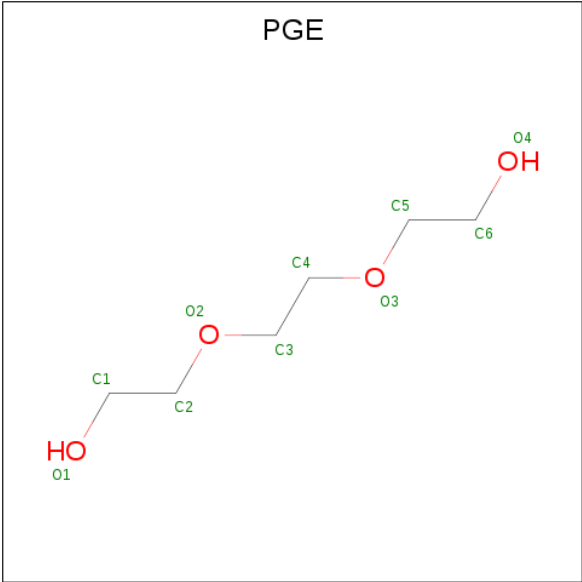
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	I	1	Total	C	O	0	0
			13	8	5		
33	I	1	Total	C	O	0	0
			13	8	5		
33	J	1	Total	C	O	0	0
			13	8	5		
33	J	1	Total	C	O	0	0
			13	8	5		
33	K	1	Total	C	O	0	0
			13	8	5		
33	U	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	X	1	Total	C	O	0	0
			13	8	5		
33	X	1	Total	C	O	0	0
			13	8	5		
33	X	1	Total	C	O	0	0
			13	8	5		
33	a	1	Total	C	O	0	0
			13	8	5		
33	a	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	c	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	c	1	Total	C	O	0	0
			13	8	5		
33	c	1	Total	C	O	0	0
			13	8	5		
33	c	1	Total	C	O	0	0
			13	8	5		
33	d	1	Total	C	O	0	0
			13	8	5		
33	e	1	Total	C	O	0	0
			13	8	5		
33	e	1	Total	C	O	0	0
			13	8	5		
33	h	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	j	1	Total	C	O	0	0
			13	8	5		
33	l	1	Total	C	O	0	0
			13	8	5		
33	x	1	Total	C	O	0	0
			13	8	5		

- Molecule 34 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			7	4	3		
34	A	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	C	1	Total	C	O	0	0
			10	6	4		
34	C	1	Total	C	O	0	0
			10	6	4		
34	D	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	I	1	Total	C	O	0	0
			10	6	4		
34	J	1	Total	C	O	0	0
			10	6	4		
34	J	1	Total	C	O	0	0
			10	6	4		
34	J	1	Total	C	O	0	0
			10	6	4		
34	O	1	Total	C	O	0	0
			10	6	4		
34	O	1	Total	C	O	0	0
			10	6	4		
34	O	1	Total	C	O	0	0
			10	6	4		
34	T	1	Total	C	O	0	0
			7	4	3		
34	V	1	Total	C	O	0	0
			10	6	4		
34	V	1	Total	C	O	0	0
			10	6	4		
34	Y	1	Total	C	O	0	0
			10	6	4		
34	a	1	Total	C	O	0	0
			10	6	4		
34	a	1	Total	C	O	0	0
			10	6	4		

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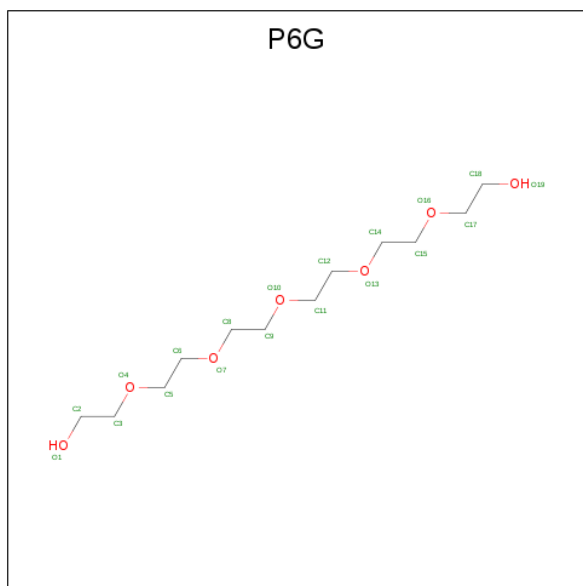
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	f	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	i	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	i	1	Total	C	O	0	0
			10	6	4		
34	j	1	Total	C	O	0	0
			10	6	4		
34	o	1	Total	C	O	0	0
			10	6	4		
34	o	1	Total	C	O	0	0
			10	6	4		
34	o	1	Total	C	O	0	0
			10	6	4		
34	t	1	Total	C	O	0	0
			10	6	4		
34	t	1	Total	C	O	0	0
			7	4	3		
34	x	1	Total	C	O	0	0
			10	6	4		

- Molecule 35 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	A	1	Total	C	O	0	0
			19	12	7		
35	A	1	Total	C	O	0	0
			19	12	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	B	1	Total	C	O	0	0
			19	12	7		
35	B	1	Total	C	O	0	0
			19	12	7		
35	C	1	Total	C	O	0	0
			19	12	7		
35	D	1	Total	C	O	0	0
			19	12	7		
35	D	1	Total	C	O	0	0
			19	12	7		
35	D	1	Total	C	O	0	0
			19	12	7		
35	E	1	Total	C	O	0	0
			19	12	7		
35	I	1	Total	C	O	0	0
			19	12	7		
35	T	1	Total	C	O	0	0
			19	12	7		
35	b	1	Total	C	O	0	0
			19	12	7		
35	b	1	Total	C	O	0	0
			19	12	7		
35	c	1	Total	C	O	0	0
			19	12	7		
35	d	1	Total	C	O	0	0
			19	12	7		
35	d	1	Total	C	O	0	0
			19	12	7		
35	j	1	Total	C	O	0	0
			19	12	7		

- Molecule 36 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	A	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	C	1	Total	C	O	0	0
			4	2	2		
36	D	1	Total	C	O	0	0
			4	2	2		
36	E	1	Total	C	O	0	0
			4	2	2		
36	E	1	Total	C	O	0	0
			4	2	2		
36	H	1	Total	C	O	0	0
			4	2	2		
36	I	1	Total	C	O	0	0
			4	2	2		
36	J	1	Total	C	O	0	0
			4	2	2		
36	O	1	Total	C	O	0	0
			4	2	2		
36	V	1	Total	C	O	0	0
			4	2	2		

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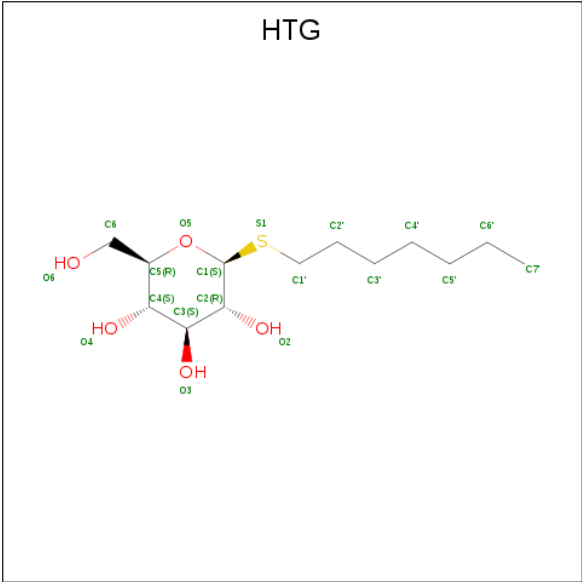
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	X	1	Total C O 4 2 2	0	0
36	a	1	Total C O 4 2 2	0	0
36	c	1	Total C O 4 2 2	0	0
36	d	1	Total C O 4 2 2	0	0
36	e	1	Total C O 4 2 2	0	0
36	i	1	Total C O 4 2 2	0	0
36	o	1	Total C O 4 2 2	0	0
36	o	1	Total C O 4 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	h	1	Total Ca 1 1	0	0
37	B	1	Total Ca 1 1	0	0
37	c	1	Total Ca 1 1	0	0
37	o	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	b	1	Total Ca 1 1	0	0

- Molecule 38 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



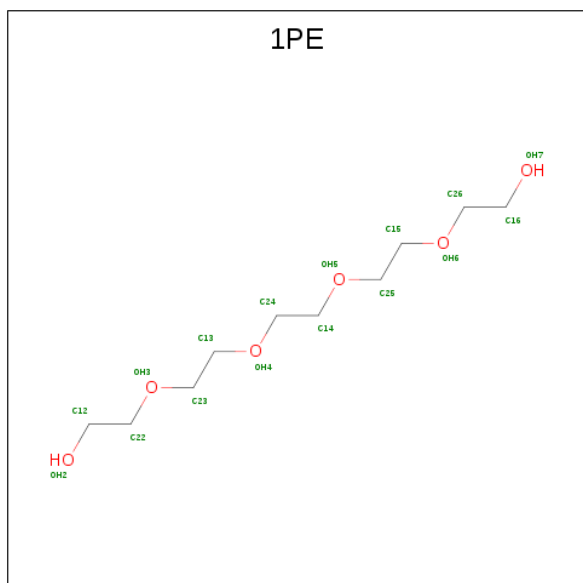
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
	B	1	Total	C	O	S		
			19	13	5	1		
	B	1	Total	C	O	S		
			19	13	5	1		
	B	1	Total	C	O	S		
			19	13	5	1		
	C	1	Total	C	O	S		
			19	13	5	1		
	C	1	Total	C	O	S		
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
	C	1	Total	C	O	S		
			19	13	5	1		
	C	1	Total	C	O	S		
			19	13	5	1		
	C	1	Total	C	O	S		
			19	13	5	1		
	C	1	Total	C	O	S		
			19	13	5	1		
	C	1	Total	C	O	S		
			19	13	5	1		
38	H	1	Total	C	O	S	0	0
			19	13	5	1		
	O	1	Total	C	O	S		
			19	13	5	1		
	V	1	Total	C	O	S		
			19	13	5	1		
	a	1	Total	C	O	S		
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	h	1	Total	C	O	S	0	0
			19	13	5	1		
38	o	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 39 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



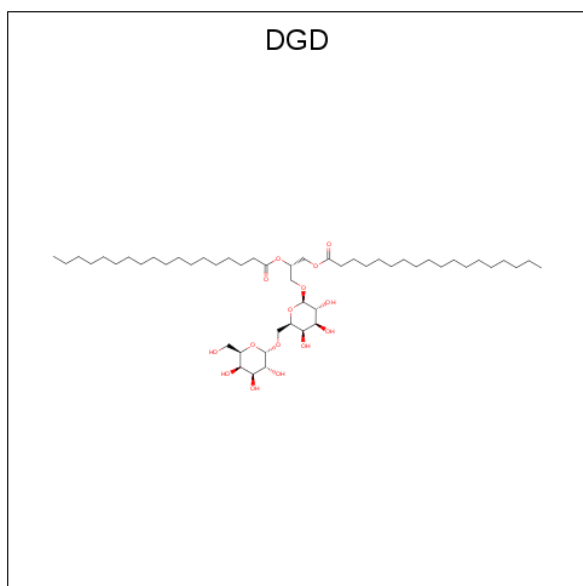
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	B	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	B	1	Total	C	O	0	0
			16	10	6		
39	L	1	Total	C	O	0	0
			16	10	6		
39	V	1	Total	C	O	0	0
			16	10	6		
39	e	1	Total	C	O	0	0
			16	10	6		
39	j	1	Total	C	O	0	0
			16	10	6		
39	x	1	Total	C	O	0	0
			16	10	6		

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



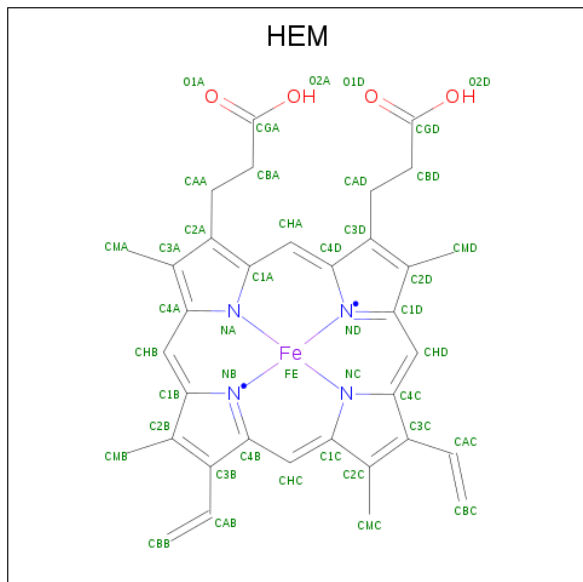
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	C	1	Total	C	O	0	0
			62	47	15		
40	C	1	Total	C	O	0	0
			56	41	15		
40	C	1	Total	C	O	0	0
			62	47	15		
40	D	1	Total	C	O	0	0
			66	51	15		
40	H	1	Total	C	O	0	0
			62	47	15		

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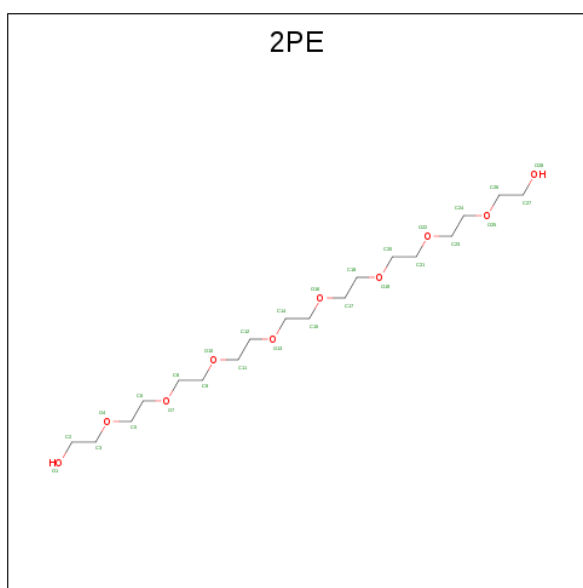
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	c	1	Total	C	O	0	0
			62	47	15		
40	c	1	Total	C	O	0	0
			57	42	15		
40	c	1	Total	C	O	0	0
			62	47	15		
40	d	1	Total	C	O	0	0
			66	51	15		
40	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	J	1	Total Mg 1 1	0	0
42	j	1	Total Mg 1 1	0	0
42	f	1	Total Mg 1 1	0	0
42	F	1	Total Mg 1 1	0	0

- Molecule 43 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	V	1	Total C O 28 18 10	0	0
43	i	1	Total C O 25 16 9	0	0

- Molecule 44 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	A	191	Total O 191 191	0	0
44	B	413	Total O 413 413	0	0
44	C	320	Total O 320 320	0	0
44	D	169	Total O 170 170	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	E	57	Total O 57 57	0	0
44	F	17	Total O 17 17	0	0
44	H	63	Total O 63 63	0	0
44	I	16	Total O 16 16	0	0
44	J	17	Total O 17 17	0	0
44	K	15	Total O 15 15	0	0
44	L	23	Total O 23 23	0	0
44	M	33	Total O 33 33	0	0
44	O	254	Total O 254 254	0	0
44	T	27	Total O 27 27	0	0
44	U	112	Total O 112 112	0	0
44	V	149	Total O 149 149	0	0
44	Y	6	Total O 6 6	0	0
44	X	10	Total O 10 10	0	0
44	Z	4	Total O 4 4	0	0
44	a	177	Total O 177 177	0	0
44	b	421	Total O 421 421	0	0
44	c	329	Total O 329 329	0	0
44	d	188	Total O 189 189	0	1
44	e	46	Total O 46 46	0	0
44	f	15	Total O 15 15	0	0

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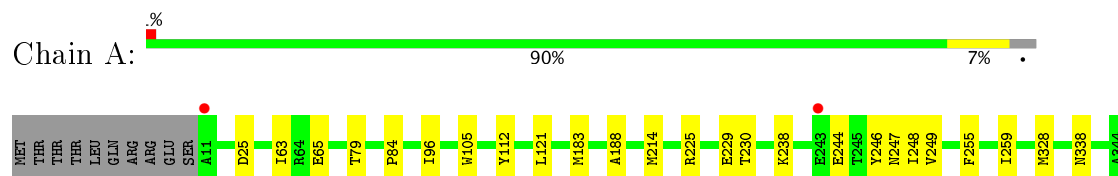
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
44	h	52	Total 52	O 52	0	0
44	i	22	Total 22	O 22	0	0
44	j	12	Total 12	O 12	0	0
44	k	9	Total 9	O 9	0	0
44	l	23	Total 23	O 23	0	0
44	m	24	Total 24	O 24	0	0
44	o	246	Total 246	O 246	0	0
44	t	17	Total 17	O 17	0	0
44	u	140	Total 140	O 140	0	0
44	v	154	Total 154	O 154	0	0
44	y	7	Total 7	O 7	0	0
44	x	8	Total 8	O 8	0	0
44	z	1	Total 1	O 1	0	0

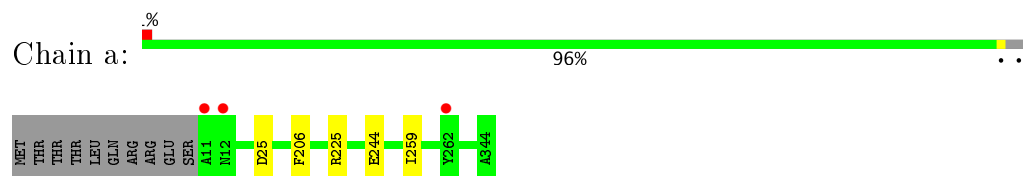
3 Residue-property plots [i](#)

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

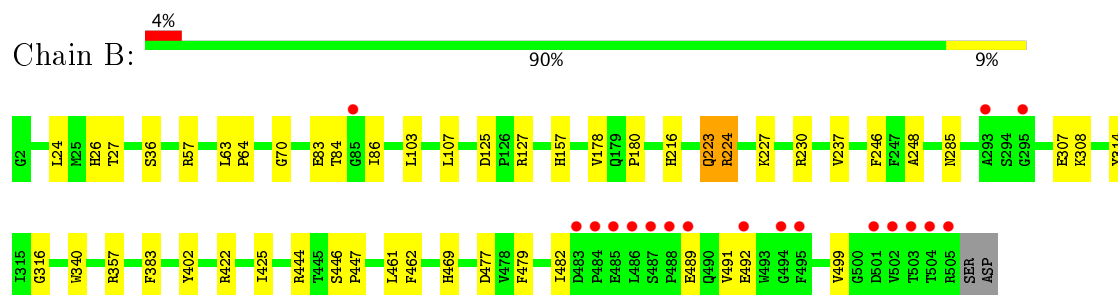
- Molecule 1: Photosystem II protein D1



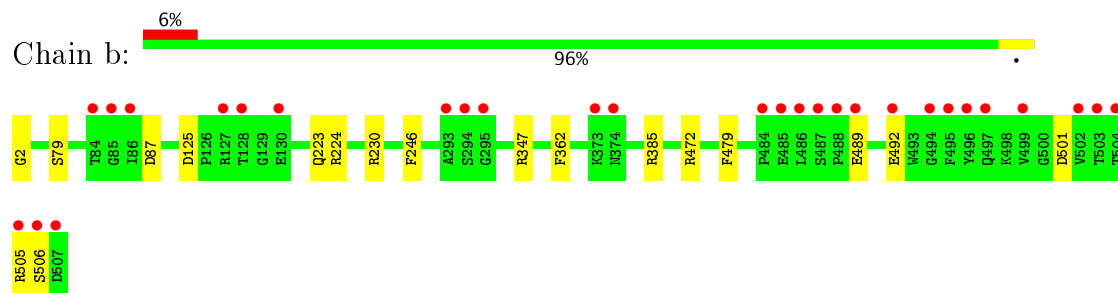
- Molecule 1: Photosystem II protein D1



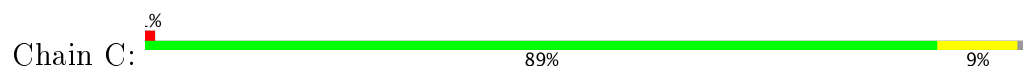
- Molecule 2: Photosystem II CP47 reaction center protein

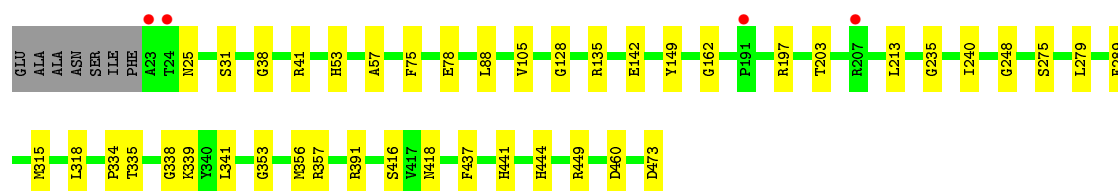


- Molecule 2: Photosystem II CP47 reaction center protein

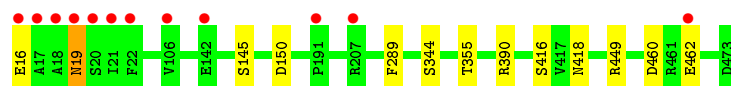


- Molecule 3: Photosystem II CP43 reaction center protein





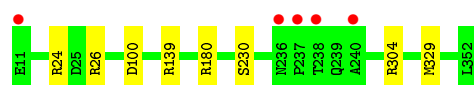
- Molecule 3: Photosystem II CP43 reaction center protein



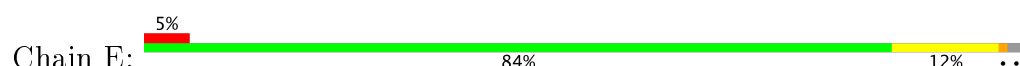
- Molecule 4: Photosystem II D2 protein



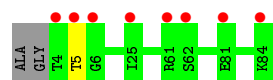
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha

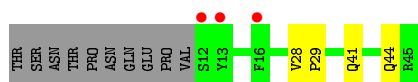


- Molecule 5: Cytochrome b559 subunit alpha

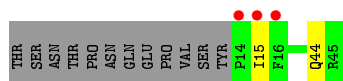


- Molecule 6: Cytochrome b559 subunit beta

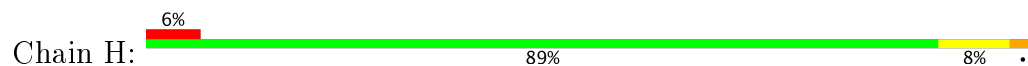




- Molecule 6: Cytochrome b559 subunit beta



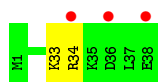
- Molecule 7: Photosystem II reaction center protein H



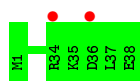
- Molecule 7: Photosystem II reaction center protein H



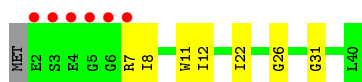
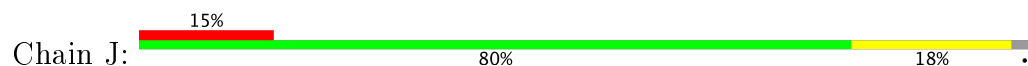
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



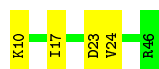
- Molecule 9: Photosystem II reaction center protein J





- Molecule 10: Photosystem II reaction center protein K

Chain K: 89% 11%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 97% .



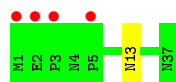
- Molecule 11: Photosystem II reaction center protein L

Chain L: 8% 84% 14% .



- Molecule 11: Photosystem II reaction center protein L

Chain l: 11% 97% .



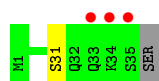
- Molecule 12: Photosystem II reaction center protein M

Chain M: 6% 78% 17% 6%



- Molecule 12: Photosystem II reaction center protein M

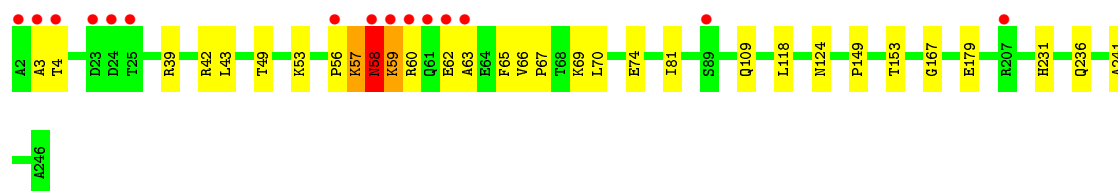
Chain m: 8% 94% . .



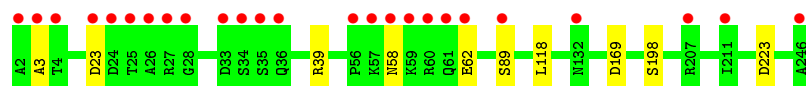
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 6% 87% 11% .

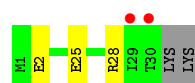
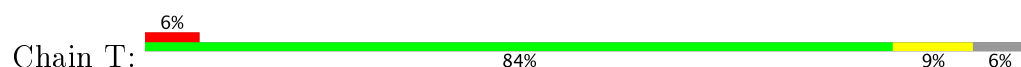




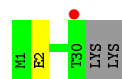
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



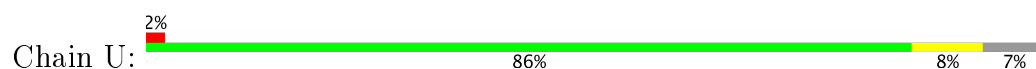
- Molecule 14: Photosystem II reaction center protein T



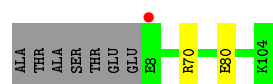
- Molecule 14: Photosystem II reaction center protein T



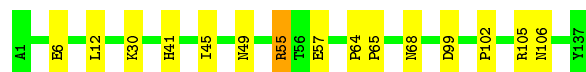
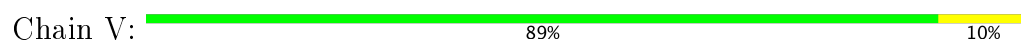
- Molecule 15: Photosystem II 12 kDa extrinsic protein



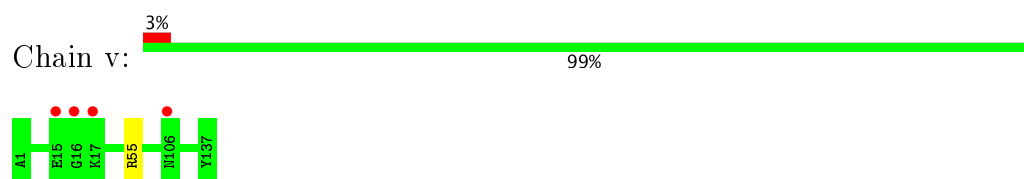
- Molecule 15: Photosystem II 12 kDa extrinsic protein



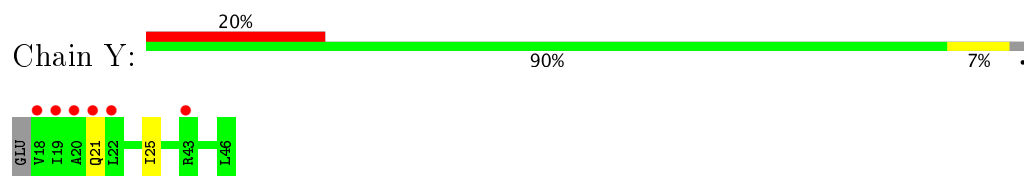
- Molecule 16: Cytochrome c-550



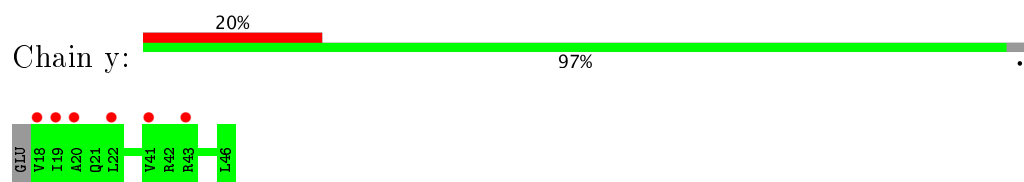
- Molecule 16: Cytochrome c-550



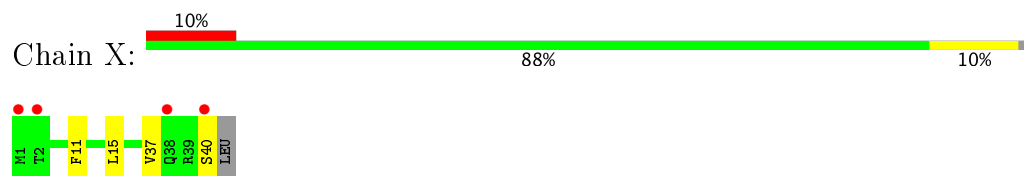
- Molecule 17: Photosystem II reaction center protein Ycf12



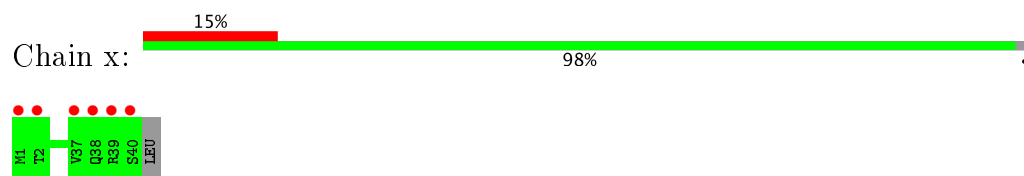
- Molecule 17: Photosystem II reaction center protein Ycf12



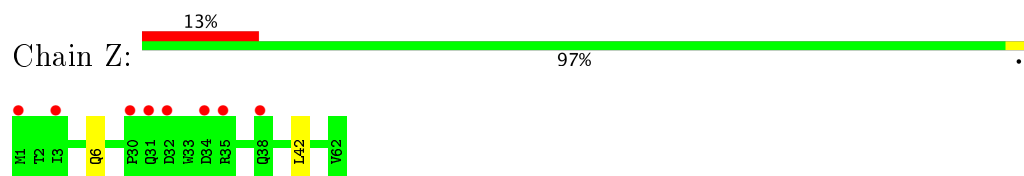
- Molecule 18: Photosystem II reaction center protein X



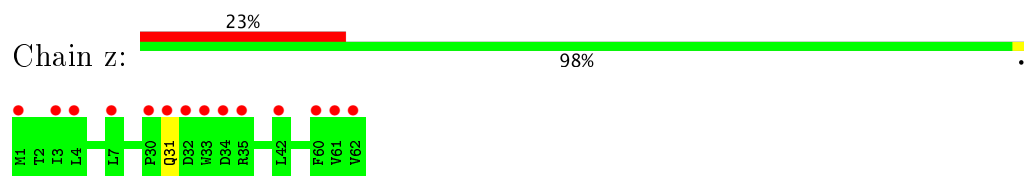
- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	178.62 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (178.62-1.90) 99.9 (20.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.092 , 0.163 0.094 , 0.164	Depositor DCC
R_{free} test set	31202 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 81.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	57584	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, 1PE, 2PE, P6G, BCT, BCR, PGE, DGD, FE2, LHG, GOL, CL, CA, CLA, PG4, HEM, FME, MHS, HTG, MG, OEX, PHO, LMT, EDO, SQD, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.99	2/2736 (0.1%)	0.88	4/3730 (0.1%)
1	a	0.93	0/2736	0.87	7/3730 (0.2%)
2	B	0.98	2/4205 (0.0%)	0.88	9/5727 (0.2%)
2	b	0.94	3/4207 (0.1%)	0.88	7/5731 (0.1%)
3	C	0.92	1/3636 (0.0%)	0.83	6/4950 (0.1%)
3	c	0.83	1/3679 (0.0%)	0.84	6/5008 (0.1%)
4	D	0.98	1/2816 (0.0%)	0.90	4/3836 (0.1%)
4	d	0.92	1/2829 (0.0%)	0.86	8/3852 (0.2%)
5	E	0.92	0/704	0.93	3/959 (0.3%)
5	e	0.86	0/693	0.83	0/944
6	F	0.84	0/284	0.71	0/387
6	f	0.74	0/265	0.74	0/360
7	H	1.01	2/544 (0.4%)	0.89	0/739
7	h	0.88	1/535 (0.2%)	0.75	0/728
8	I	0.90	0/311	0.81	0/419
8	i	0.86	0/311	0.83	0/419
9	J	0.87	0/306	0.74	0/413
9	j	0.75	0/287	0.77	0/388
10	K	0.80	0/303	0.75	0/416
10	k	0.75	0/303	0.77	0/416
11	L	1.00	1/319 (0.3%)	0.93	0/433
11	l	0.93	0/328	0.87	0/446
12	M	0.99	0/279	0.83	0/380
12	m	0.98	1/275 (0.4%)	0.88	0/375
13	O	0.90	0/1953	0.92	1/2649 (0.0%)
13	o	0.90	1/1948 (0.1%)	0.94	6/2641 (0.2%)
14	T	1.21	1/266 (0.4%)	1.06	1/362 (0.3%)
14	t	1.07	2/266 (0.8%)	0.91	0/362
15	U	0.85	0/803	0.92	2/1088 (0.2%)
15	u	0.98	1/785 (0.1%)	0.90	0/1064
16	V	0.95	3/1104 (0.3%)	0.89	3/1498 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.86	0/1096	0.84	4/1487 (0.3%)
17	Y	0.76	0/223	0.80	0/299
17	y	0.71	0/224	0.83	0/299
18	X	0.77	0/306	0.82	0/413
18	x	0.83	0/298	0.83	0/402
19	Z	0.74	0/490	0.79	0/669
19	z	0.73	0/490	0.70	0/669
All	All	0.92	24/43143 (0.1%)	0.87	71/58688 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	66	GLY	C-O	7.92	1.36	1.23
7	H	66	GLY	C-OXT	7.84	1.38	1.23
14	t	2	GLU	CB-CG	-7.21	1.38	1.52
15	u	80	GLU	CD-OE2	-6.83	1.18	1.25
16	V	57	GLU	CG-CD	6.71	1.62	1.51
1	A	65	GLU	CD-OE2	6.36	1.32	1.25
16	V	6	GLU	CG-CD	6.25	1.61	1.51
14	t	2	GLU	CD-OE2	-6.12	1.19	1.25
13	o	198	SER	CB-OG	-6.09	1.34	1.42
16	V	57	GLU	CD-OE1	6.09	1.32	1.25
7	h	61	SER	CB-OG	-6.06	1.34	1.42
2	B	307	GLU	CD-OE2	-5.91	1.19	1.25
14	T	2	GLU	CD-OE2	-5.74	1.19	1.25
12	m	31	SER	CB-OG	5.64	1.49	1.42
2	b	2	GLY	N-CA	5.58	1.54	1.46
3	c	344	SER	CB-OG	5.51	1.49	1.42
3	C	275	SER	CB-OG	5.46	1.49	1.42
4	D	310	GLU	CD-OE2	-5.39	1.19	1.25
1	A	244	GLU	CD-OE1	5.31	1.31	1.25
2	B	340	TRP	CE2-CZ2	-5.15	1.30	1.39
11	L	11	GLU	CD-OE1	5.06	1.31	1.25
2	b	347[A]	ARG	CZ-NH2	-5.06	1.26	1.33
2	b	347[B]	ARG	CZ-NH2	-5.06	1.26	1.33
4	d	230	SER	CB-OG	5.04	1.48	1.42

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	139	ARG	NE-CZ-NH1	14.27	127.43	120.30
4	D	139	ARG	NE-CZ-NH2	-9.74	115.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	357	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	a	225[A]	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	a	225[B]	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	a	225[A]	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	a	225[B]	ARG	NE-CZ-NH2	-8.60	116.00	120.30
4	d	100	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	225[A]	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	A	225[B]	ARG	NE-CZ-NH1	-7.49	116.56	120.30
2	B	444	ARG	NE-CZ-NH2	-7.49	116.56	120.30
3	C	460	ASP	CB-CG-OD1	7.47	125.02	118.30
2	B	224	ARG	NE-CZ-NH2	7.46	124.03	120.30
4	d	139	ARG	NE-CZ-NH2	-7.26	116.67	120.30
2	b	385	ARG	NE-CZ-NH2	-7.14	116.73	120.30
2	B	224	ARG	NE-CZ-NH1	-7.07	116.76	120.30
13	o	39[A]	ARG	NE-CZ-NH1	7.04	123.82	120.30
13	o	39[B]	ARG	NE-CZ-NH1	7.04	123.82	120.30
3	c	460	ASP	CB-CG-OD1	6.97	124.57	118.30
4	d	139	ARG	NE-CZ-NH1	6.90	123.75	120.30
3	c	390	ARG	NE-CZ-NH1	6.86	123.73	120.30
13	O	39	ARG	NE-CZ-NH2	6.70	123.65	120.30
2	b	224	ARG	NE-CZ-NH1	-6.61	117.00	120.30
2	B	444	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	25	ASP	CB-CG-OD2	-6.37	112.57	118.30
2	b	125	ASP	CB-CG-OD1	6.28	123.95	118.30
13	o	39[A]	ARG	NE-CZ-NH2	-6.09	117.25	120.30
13	o	39[B]	ARG	NE-CZ-NH2	-6.09	117.25	120.30
14	T	28	ARG	NE-CZ-NH2	6.05	123.33	120.30
4	D	100	ASP	CB-CG-OD1	5.98	123.68	118.30
16	v	55[A]	ARG	NE-CZ-NH1	5.97	123.28	120.30
16	v	55[B]	ARG	NE-CZ-NH1	5.97	123.28	120.30
13	o	223	ASP	CB-CG-OD1	5.92	123.63	118.30
4	d	24	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	a	25	ASP	CB-CG-OD2	-5.84	113.04	118.30
3	C	473	ASP	CB-CG-OD1	5.82	123.53	118.30
1	a	25	ASP	CB-CG-OD1	5.76	123.48	118.30
16	v	55[A]	ARG	NE-CZ-NH2	-5.75	117.43	120.30
16	v	55[B]	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	b	230	ARG	NE-CZ-NH1	5.72	123.16	120.30
16	V	55[A]	ARG	NE-CZ-NH1	5.69	123.14	120.30
16	V	55[B]	ARG	NE-CZ-NH1	5.69	123.14	120.30
5	E	51	ARG	NE-CZ-NH1	5.68	123.14	120.30
4	D	24	ARG	NE-CZ-NH2	-5.62	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	87	ASP	CB-CG-OD1	5.59	123.33	118.30
2	b	224	ARG	NE-CZ-NH2	5.55	123.08	120.30
4	d	304	ARG	NE-CZ-NH1	5.52	123.06	120.30
3	C	197	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	25	ASP	CB-CG-OD1	5.49	123.24	118.30
3	C	473	ASP	CB-CG-OD2	-5.48	113.37	118.30
2	B	357	ARG	NE-CZ-NH2	-5.47	117.56	120.30
3	c	449	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	B	477	ASP	CB-CG-OD1	5.45	123.21	118.30
3	c	460	ASP	CB-CG-OD2	-5.45	113.40	118.30
3	c	390	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	a	206	PHE	CB-CG-CD1	5.42	124.59	120.80
4	d	26	ARG	NE-CZ-NH1	5.41	123.01	120.30
3	C	357	ARG	NE-CZ-NH2	-5.41	117.60	120.30
3	C	357	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	B	402	TYR	CZ-CE2-CD2	-5.38	114.96	119.80
16	V	99	ASP	CB-CG-OD1	5.38	123.14	118.30
15	U	39	ARG	NE-CZ-NH1	5.35	122.98	120.30
2	B	230	ARG	NE-CZ-NH1	5.33	122.97	120.30
4	d	24	ARG	NE-CZ-NH2	-5.31	117.65	120.30
5	E	45	ASP	CB-CG-OD1	5.30	123.07	118.30
15	U	97	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	b	501	ASP	CB-CG-OD1	5.25	123.03	118.30
4	d	100	ASP	CB-CG-OD2	-5.23	113.60	118.30
3	c	150	ASP	CB-CG-OD1	5.09	122.89	118.30
5	E	63	ILE	CG1-CB-CG2	-5.07	100.24	111.40
13	o	169	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2639	0	2551	20	0
1	a	2639	0	2551	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4032	0	3914	46	0
2	b	4037	0	3915	0	0
3	C	3508	0	3440	35	0
3	c	3553	0	3474	0	0
4	D	2731	0	2637	27	0
4	d	2741	0	2647	0	0
5	E	676	0	671	10	0
5	e	668	0	658	0	0
6	F	275	0	282	2	0
6	f	257	0	269	0	0
7	H	525	0	558	8	0
7	h	519	0	545	0	0
8	I	314	0	328	3	0
8	i	314	0	328	0	0
9	J	294	0	309	8	0
9	j	281	0	285	0	0
10	K	293	0	305	5	0
10	k	293	0	305	0	0
11	L	309	0	327	4	0
11	l	315	0	335	0	0
12	M	286	0	303	23	0
12	m	289	0	310	0	0
13	O	1904	0	1887	23	0
13	o	1902	0	1885	0	0
14	T	271	0	277	2	0
14	t	271	0	277	0	0
15	U	786	0	787	3	0
15	u	774	0	773	0	0
16	V	1077	0	1092	11	0
16	v	1072	0	1086	0	0
17	Y	219	0	253	2	0
17	y	220	0	255	0	0
18	X	300	0	340	5	0
18	x	295	0	329	0	0
19	Z	479	0	516	0	0
19	z	479	0	516	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	V	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	2	0	0	0	0
22	v	1	0	0	0	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
23	m	8	0	2	0	0
24	A	190	0	203	8	0
24	B	1015	0	1093	48	0
24	C	835	0	910	37	0
24	D	195	0	216	10	0
24	a	190	0	203	0	0
24	b	1025	0	1116	0	0
24	c	835	0	910	0	0
24	d	195	0	216	0	0
25	A	64	0	74	2	0
25	D	64	0	74	3	0
25	a	64	0	74	0	0
25	d	64	0	74	0	0
26	A	40	0	56	3	0
26	B	120	0	168	14	0
26	C	120	0	168	7	0
26	D	40	0	56	4	0
26	H	40	0	56	3	0
26	K	40	0	56	6	0
26	T	40	0	56	9	0
26	a	40	0	56	0	0
26	b	120	0	168	0	0
26	c	120	0	168	0	0
26	d	40	0	56	0	0
26	h	40	0	56	0	0
26	k	40	0	56	0	0
26	t	40	0	56	0	0
27	A	55	0	80	6	0
27	D	55	0	80	0	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	162	0	234	5	0
28	F	54	0	78	0	0
28	a	162	0	234	0	0
28	b	54	0	78	0	0
28	h	54	0	78	0	0
28	l	54	0	78	0	0
28	x	54	0	78	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	51	0	72	3	0
29	B	106	0	158	9	0
29	C	157	0	230	4	0
29	J	47	0	64	0	0
29	a	51	0	72	0	0
29	b	51	0	72	0	0
29	c	102	0	144	0	0
29	d	55	0	86	0	0
29	j	47	0	64	0	0
29	z	55	0	86	0	0
30	A	12	0	16	4	0
30	B	42	0	56	1	0
30	C	24	0	31	13	0
30	D	18	0	24	2	0
30	F	6	0	8	0	0
30	O	30	0	40	2	0
30	T	12	0	16	2	0
30	U	6	0	8	2	0
30	V	30	0	40	0	0
30	a	12	0	16	0	0
30	b	36	0	48	0	0
30	c	24	0	32	0	0
30	d	12	0	16	0	0
30	e	6	0	8	0	0
30	f	12	0	16	0	0
30	m	6	0	8	0	0
30	o	18	0	24	0	0
30	t	6	0	8	0	0
30	u	12	0	16	0	0
30	v	30	0	40	0	0
30	y	6	0	8	0	0
31	A	35	0	46	0	0
31	B	35	0	46	2	0
31	C	35	0	46	0	0
31	F	35	0	46	0	0
31	I	35	0	46	1	0
31	J	35	0	46	1	0
31	M	70	0	92	1	0
31	Y	35	0	46	1	0
31	a	35	0	46	0	0
31	b	35	0	46	0	0
31	c	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	f	35	0	46	0	0
31	j	35	0	46	0	0
31	m	70	0	92	0	0
31	t	35	0	46	0	0
31	u	35	0	46	0	0
32	A	42	0	54	0	0
32	B	49	0	74	0	0
32	D	147	0	222	2	0
32	E	42	0	57	2	0
32	a	41	0	52	0	0
32	d	147	0	222	0	0
32	e	42	0	57	0	0
32	l	49	0	74	0	0
33	A	13	0	18	0	0
33	B	104	0	144	0	0
33	C	65	0	90	0	0
33	D	13	0	18	0	0
33	E	26	0	36	0	0
33	H	52	0	72	4	0
33	I	39	0	54	2	0
33	J	26	0	36	0	0
33	K	13	0	18	0	0
33	U	13	0	18	0	0
33	V	65	0	90	0	0
33	X	39	0	54	0	0
33	a	26	0	36	0	0
33	b	52	0	72	0	0
33	c	52	0	72	0	0
33	d	13	0	18	0	0
33	e	26	0	36	0	0
33	h	13	0	18	0	0
33	i	52	0	72	0	0
33	j	13	0	18	0	0
33	l	13	0	18	0	0
33	x	13	0	18	0	0
34	A	17	0	23	0	0
34	B	70	0	98	2	0
34	C	20	0	28	0	0
34	D	10	0	14	0	0
34	E	60	0	84	0	0
34	H	40	0	56	0	0
34	I	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	J	30	0	42	0	0
34	O	30	0	42	5	0
34	T	7	0	9	0	0
34	V	20	0	28	0	0
34	Y	10	0	14	0	0
34	a	20	0	28	0	0
34	b	100	0	140	0	0
34	c	50	0	70	0	0
34	f	10	0	14	0	0
34	h	40	0	56	0	0
34	i	20	0	28	0	0
34	j	10	0	14	0	0
34	o	40	0	56	0	0
34	t	17	0	23	0	0
34	x	10	0	14	0	0
35	A	38	0	52	0	0
35	B	38	0	52	1	0
35	C	19	0	26	3	0
35	D	57	0	78	0	0
35	E	19	0	26	0	0
35	I	19	0	26	0	0
35	T	19	0	26	2	0
35	b	38	0	52	0	0
35	c	19	0	26	0	0
35	d	38	0	52	0	0
35	j	19	0	26	0	0
36	A	4	0	6	0	0
36	B	16	0	24	0	0
36	C	4	0	6	0	0
36	D	4	0	6	3	0
36	E	8	0	12	0	0
36	H	4	0	6	0	0
36	I	4	0	6	0	0
36	J	4	0	6	0	0
36	O	4	0	6	0	0
36	V	4	0	6	0	0
36	X	4	0	6	0	0
36	a	4	0	6	0	0
36	c	4	0	6	0	0
36	d	4	0	6	0	0
36	e	4	0	6	0	0
36	i	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	o	8	0	12	0	0
37	B	1	0	0	0	0
37	O	1	0	0	0	0
37	b	1	0	0	0	0
37	c	1	0	0	0	0
37	h	1	0	0	0	0
37	o	1	0	0	0	0
38	B	76	0	104	3	0
38	C	114	0	156	4	0
38	H	19	0	26	1	0
38	O	19	0	26	0	0
38	V	19	0	26	0	0
38	a	19	0	26	0	0
38	b	76	0	104	0	0
38	c	76	0	104	0	0
38	h	19	0	26	0	0
38	o	19	0	26	0	0
39	B	32	0	44	0	0
39	L	16	0	22	0	0
39	V	16	0	22	0	0
39	e	16	0	22	0	0
39	j	16	0	22	0	0
39	x	16	0	22	0	0
40	C	180	0	234	0	0
40	D	66	0	96	2	0
40	H	62	0	82	0	0
40	c	181	0	236	0	0
40	d	66	0	96	0	1
40	h	62	0	82	0	0
41	E	43	0	30	5	0
41	V	43	0	30	0	0
41	e	43	0	30	0	0
41	v	43	0	30	0	0
42	F	1	0	0	0	0
42	J	1	0	0	0	0
42	f	1	0	0	0	0
42	j	1	0	0	0	0
43	V	28	0	38	3	0
43	i	25	0	33	0	0
44	A	191	0	0	6	0
44	B	413	0	0	13	0
44	C	320	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	D	170	0	0	7	0
44	E	57	0	0	3	0
44	F	17	0	0	0	0
44	H	63	0	0	3	0
44	I	16	0	0	3	0
44	J	17	0	0	2	0
44	K	15	0	0	0	0
44	L	23	0	0	0	0
44	M	33	0	0	2	0
44	O	254	0	0	12	0
44	T	27	0	0	1	0
44	U	112	0	0	3	0
44	V	149	0	0	7	0
44	X	10	0	0	0	0
44	Y	6	0	0	0	0
44	Z	4	0	0	0	0
44	a	177	0	0	0	0
44	b	421	0	0	0	0
44	c	329	0	0	0	0
44	d	189	0	0	0	0
44	e	46	0	0	0	0
44	f	15	0	0	0	0
44	h	52	0	0	0	0
44	i	22	0	0	0	0
44	j	12	0	0	0	0
44	k	9	0	0	0	0
44	l	23	0	0	0	0
44	m	24	0	0	0	0
44	o	246	0	0	0	0
44	t	17	0	0	0	0
44	u	140	0	0	0	0
44	v	154	0	0	0	1
44	x	8	0	0	0	0
44	y	7	0	0	0	0
44	z	1	0	0	0	0
All	All	57584	0	56552	376	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (376) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:16[B]:LEU:CD2	12:M:16[B]:LEU:HD11	2.62	1.41
12:M:16[B]:LEU:HD22	12:M:16[B]:LEU:CD1	2.67	1.22
12:M:16[B]:LEU:HD13	12:M:16[B]:LEU:HD13	0.00	1.10
12:M:16[B]:LEU:HD21	12:M:16[B]:LEU:HD21	0.00	1.05
12:M:16[B]:LEU:CD2	12:M:16[B]:LEU:CD1	2.46	1.05
12:M:16[B]:LEU:HD21	12:M:16[B]:LEU:CD2	0.97	1.04
4:D:301:GLN:OE1	44:D:501:HOH:O	1.76	1.03
2:B:127[B]:ARG:CG	2:B:127[B]:ARG:HH21	1.73	1.01
38:B:623:HTG:H61	44:O:427:HOH:O	1.64	0.97
1:A:214:MET:HG2	27:A:611:PL9:H102	1.45	0.97
3:C:338:GLY:O	30:C:528:GOL:H32	1.63	0.97
2:B:127[B]:ARG:HG3	2:B:127[B]:ARG:HH21	0.82	0.96
12:M:16[B]:LEU:CD1	12:M:16[B]:LEU:HD13	0.97	0.96
2:B:127[B]:ARG:HG3	2:B:127[B]:ARG:NH2	1.64	0.96
30:A:614:GOL:O2	44:A:701:HOH:O	1.85	0.93
12:M:16[B]:LEU:HD22	12:M:16[B]:LEU:HD11	2.92	0.89
22:V:202:CL:CL	44:V:390:HOH:O	2.27	0.88
12:M:16[B]:LEU:CD1	12:M:16[B]:LEU:CD1	0.00	0.86
35:C:541:P6G:O13	35:C:541:P6G:H172	5.48	0.85
26:T:102:BCR:H382	26:T:102:BCR:H23C	1.62	0.81
30:C:528:GOL:O3	44:C:601:HOH:O	1.96	0.81
24:B:607:CLA:HBB1	24:B:607:CLA:HMB1	1.63	0.80
30:A:615:GOL:C3	44:E:201:HOH:O	2.30	0.79
24:D:405:CLA:H192	18:X:15[A]:LEU:HD11	1.65	0.79
10:K:17:ILE:H	10:K:17:ILE:HD12	1.48	0.78
24:C:505:CLA:HBB1	24:C:505:CLA:HMB1	1.84	0.78
1:A:338:ASN:HD21	30:C:528:GOL:H31	1.50	0.77
8:I:33:LYS:HG2	44:I:213:HOH:O	1.85	0.77
4:D:11:GLU:N	36:D:419:EDO:HO2	1.83	0.77
30:A:615:GOL:H31	44:E:201:HOH:O	1.83	0.76
12:M:33:GLN:HG2	12:M:33:GLN:HB2	2.83	0.76
24:C:506:CLA:HBB1	24:C:506:CLA:HMB1	1.66	0.76
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.66	0.76
4:D:316:THR:HG21	44:D:561:HOH:O	1.85	0.76
38:C:531:HTG:O6	44:C:602:HOH:O	2.03	0.76
24:D:405:CLA:HBB1	24:D:405:CLA:HMB1	1.72	0.76
4:D:336:MHS:HM3	44:D:611:HOH:O	1.87	0.75
24:C:503:CLA:HBB1	24:C:503:CLA:HMB1	1.77	0.74
12:M:4:ASN:ND2	44:M:201:HOH:O	2.25	0.73
25:D:401:PHO:HBB1	25:D:401:PHO:HMB1	1.77	0.73
2:B:83:GLU:O	44:B:701:HOH:O	2.06	0.73
24:C:512:CLA:HMB1	24:C:512:CLA:HBB1	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:A:756:HOH:O	30:C:528:GOL:H11	1.90	0.70
24:C:506:CLA:HMC2	24:C:507:CLA:H102	1.73	0.70
24:D:403:CLA:HBB1	24:D:403:CLA:HMB1	1.74	0.70
24:C:510:CLA:HBB1	24:C:510:CLA:HMB1	1.73	0.70
26:T:102:BCR:H311	26:T:102:BCR:HC8	1.72	0.69
24:B:609:CLA:HMB1	24:B:609:CLA:HBB1	1.92	0.68
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	1.75	0.68
16:V:68:ASN:HD21	43:V:216:2PE:H261	1.57	0.68
34:O:308:PGE:H22	44:O:482:HOH:O	19.20	0.68
24:B:616:CLA:HMB1	24:B:616:CLA:HBB1	1.81	0.68
25:A:608:PHO:HMB1	25:A:608:PHO:HBB1	1.77	0.67
12:M:33:GLN:HB2	12:M:33:GLN:CG	2.05	0.66
35:C:541:P6G:C12	35:C:541:P6G:H172	6.70	0.66
38:C:529:HTG:H7'2	31:I:101:LMT:H123	1.78	0.66
1:A:248:ILE:HD11	44:A:848:HOH:O	1.95	0.65
1:A:249:VAL:HG12	2:B:491:VAL:HG21	1.79	0.65
24:A:606:CLA:HMB1	24:A:606:CLA:HBB1	1.77	0.65
2:B:491:VAL:HG12	4:D:136[A]:VAL:HG13	1.79	0.65
26:D:406:BCR:C8	26:D:406:BCR:H331	2.26	0.65
44:A:701:HOH:O	13:O:109:GLN:NE2	2.30	0.65
1:A:338:ASN:ND2	30:C:528:GOL:H31	2.12	0.65
24:B:612:CLA:HMB1	24:B:612:CLA:HBB1	1.79	0.65
16:V:64:PRO:HB2	43:V:216:2PE:H241	1.80	0.64
24:B:611:CLA:HBB1	24:B:611:CLA:HHC	1.79	0.64
24:C:508:CLA:HBB1	24:C:508:CLA:HMB1	1.82	0.64
16:V:12:LEU:HD22	44:V:305:HOH:O	24.91	0.63
24:C:511:CLA:HBB1	24:C:511:CLA:HMB1	1.86	0.63
29:B:621:LMG:H291	44:B:903:HOH:O	31.71	0.63
24:B:603:CLA:HBB1	24:B:603:CLA:HMB1	1.79	0.63
24:B:615:CLA:HBB1	24:B:615:CLA:HMB1	1.95	0.63
8:I:34:ARG:NH2	44:I:201:HOH:O	20.75	0.63
7:H:12[B]:ARG:NH2	44:H:201:HOH:O	66.19	0.62
30:A:615:GOL:H32	44:E:201:HOH:O	1.97	0.62
24:B:610:CLA:HBB1	24:B:610:CLA:HMB1	1.80	0.62
40:D:408:DGD:HBG1	30:D:412:GOL:O3	1.99	0.61
24:C:507:CLA:HMB1	24:C:507:CLA:HBB1	2.02	0.61
24:C:513:CLA:HMB1	24:C:513:CLA:HBB1	1.87	0.61
24:B:604:CLA:C4D	24:B:606:CLA:H43	2.30	0.61
1:A:183:MET:HA	24:A:606:CLA:HMD2	1.82	0.61
13:O:70:LEU:HD22	34:O:308:PGE:H62	1.82	0.61
24:A:609:CLA:H203	24:C:506:CLA:H142	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:231:HIS:ND1	44:O:405:HOH:O	17.49	0.60
26:B:620:BCR:H331	26:B:620:BCR:HC8	1.83	0.60
24:B:602:CLA:HHC	24:B:602:CLA:HBB1	1.84	0.60
2:B:462:PHE:CE2	24:B:614:CLA:HMB3	2.42	0.60
26:B:619:BCR:C8	26:B:619:BCR:H331	2.32	0.60
24:B:602:CLA:H92	26:H:102:BCR:H403	1.84	0.59
10:K:24:VAL:HG13	17:Y:25:ILE:HD13	2.05	0.59
12:M:16[B]:LEU:HD21	12:M:16[B]:LEU:CG	2.06	0.59
4:D:336:MHS:HM3	44:D:622:HOH:O	45.33	0.59
24:B:604:CLA:HMB1	24:B:604:CLA:HBB1	1.94	0.59
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.38	0.59
9:J:7[B]:ARG:NH2	44:J:201:HOH:O	2.35	0.59
24:A:609:CLA:HBB1	24:A:609:CLA:HMB1	1.84	0.59
2:B:57:ARG:NH1	44:B:701:HOH:O	20.75	0.59
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.38	0.59
26:A:610:BCR:C8	26:A:610:BCR:H331	2.32	0.59
24:C:504:CLA:C15	32:D:411:LHG:C38	2.81	0.59
26:H:102:BCR:H331	26:H:102:BCR:C8	2.32	0.59
12:M:16[B]:LEU:CD2	12:M:16[B]:LEU:CD2	0.00	0.59
24:C:502:CLA:HBB1	24:C:502:CLA:HMB1	2.03	0.59
24:B:602:CLA:H11	24:B:602:CLA:C7	2.33	0.58
24:B:611:CLA:H192	24:B:611:CLA:H152	2.14	0.58
31:B:622:LMT:H122	29:B:634:LMG:H453	1.85	0.58
24:B:602:CLA:H141	34:B:646:PGE:C6	2.33	0.58
24:B:605:CLA:HMB1	24:B:605:CLA:HBB1	1.92	0.58
35:C:541:P6G:O13	35:C:541:P6G:C17	4.94	0.58
40:D:408:DGD:HD61	5:E:45:ASP:HB3	1.85	0.58
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.12	0.58
30:C:523:GOL:C3	44:V:308:HOH:O	2.52	0.57
27:A:611:PL9:H502	4:D:39:PRO:HG3	1.86	0.57
7:H:65:LEU:HB2	7:H:66:GLY:HA2	1.84	0.57
1:A:338:ASN:HD21	30:C:528:GOL:C3	2.17	0.57
13:O:57:LYS:O	13:O:59:LYS:N	2.37	0.57
2:B:216:HIS:CE1	24:B:610:CLA:NA	2.73	0.57
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	1.96	0.57
2:B:180:PRO:HB2	35:B:652:P6G:H32	1.86	0.56
26:T:102:BCR:C23	26:T:102:BCR:H382	2.39	0.56
3:C:339:LYS:O	44:C:602:HOH:O	63.37	0.56
2:B:223[A]:GLN:NE2	44:B:706:HOH:O	2.38	0.56
13:O:70:LEU:CD2	34:O:308:PGE:H62	2.35	0.56
24:B:617:CLA:HMB1	24:B:617:CLA:HBB1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:GLU:HG2	44:C:635:HOH:O	2.04	0.56
24:B:602:CLA:H141	34:B:646:PGE:H62	1.87	0.56
8:I:33:LYS:HE2	44:I:213:HOH:O	2.05	0.56
3:C:437:PHE:CE2	24:C:510:CLA:HMB3	2.44	0.56
24:A:607:CLA:HBB1	24:A:607:CLA:HMB1	1.87	0.56
24:B:602:CLA:H93	33:H:106:PG4:H11	1.88	0.55
2:B:127[A]:ARG:NH1	44:B:707:HOH:O	2.38	0.55
26:B:618:BCR:H23C	26:B:618:BCR:H382	1.87	0.55
2:B:103:LEU:HD21	24:B:606:CLA:HMC3	1.87	0.55
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.41	0.55
3:C:437:PHE:CZ	24:C:510:CLA:HMB3	2.40	0.55
26:B:620:BCR:C8	26:B:620:BCR:H331	2.36	0.55
24:B:608:CLA:H42	29:B:621:LMG:H302	2.11	0.55
30:C:523:GOL:H31	44:V:308:HOH:O	2.06	0.55
7:H:12[A]:ARG:HG2	44:H:251:HOH:O	2.06	0.55
2:B:462:PHE:CZ	24:B:614:CLA:HMB3	2.56	0.54
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.70	0.54
13:O:59:LYS:NZ	44:O:407:HOH:O	2.40	0.54
24:D:405:CLA:H192	18:X:15[A]:LEU:CD1	2.34	0.54
33:H:106:PG4:H51	33:H:106:PG4:O2	2.07	0.54
10:K:17:ILE:H	10:K:17:ILE:CD1	2.18	0.54
26:H:102:BCR:H331	26:H:102:BCR:HC8	1.87	0.54
2:B:127[B]:ARG:CG	2:B:127[B]:ARG:NH2	2.46	0.54
2:B:248:ALA:HA	24:B:604:CLA:H42	2.02	0.54
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.38	0.54
24:C:501:CLA:H192	24:C:506:CLA:C1B	2.50	0.53
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.91	0.53
1:A:246:TYR:OH	44:A:702:HOH:O	2.18	0.53
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.22	0.53
24:C:502:CLA:H61	24:C:512:CLA:H42	1.99	0.53
30:D:402:GOL:H11	12:M:1:FME:HG2	1.89	0.53
13:O:56:PRO:HG3	13:O:63:ALA:HB2	2.20	0.53
24:C:501:CLA:H42	24:C:502:CLA:HMD1	2.06	0.52
3:C:78:GLU:OE2	16:V:106[A]:ASN:ND2	2.42	0.52
29:A:613:LMG:C43	29:A:613:LMG:H242	2.39	0.52
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.15	0.52
7:H:25:TRP:CD1	38:H:101:HTG:H1	2.99	0.52
24:B:602:CLA:H41	44:B:1040:HOH:O	62.11	0.52
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	2.06	0.52
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.90	0.52
30:T:103:GOL:H32	35:T:105:P6G:H151	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:602:CLA:H11	24:B:602:CLA:H71	1.92	0.52
2:B:499:VAL:HG12	4:D:135:LEU:HB3	2.25	0.52
12:M:20:VAL:HG11	12:M:20:VAL:HG22	3.11	0.51
24:B:605:CLA:HMD2	24:B:613:CLA:H203	2.14	0.51
12:M:16[B]:LEU:CD2	12:M:16[B]:LEU:CG	1.52	0.51
9:J:11:TRP:CZ2	9:J:12:ILE:HD11	3.24	0.51
10:K:17:ILE:N	10:K:17:ILE:HD12	2.21	0.51
3:C:338:GLY:O	30:C:528:GOL:C3	2.49	0.51
26:K:101:BCR:H382	26:K:101:BCR:C23	2.52	0.51
24:D:404:CLA:HBC3	24:D:404:CLA:HHD	1.99	0.51
29:B:634:LMG:H201	4:D:32:TRP:CE3	2.46	0.51
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.53	0.51
13:O:124:ASN:O	30:O:305:GOL:H12	2.10	0.51
26:C:525:BCR:H331	26:C:525:BCR:C8	2.40	0.51
3:C:135:ARG:NE	29:C:526:LMG:O5	2.37	0.51
44:B:754:HOH:O	7:H:64:ALA:HB1	51.35	0.50
24:C:502:CLA:H193	38:C:521:HTG:H3'1	1.94	0.50
13:O:179:GLU:HG2	44:O:620:HOH:O	2.11	0.50
38:B:623:HTG:C6	44:O:427:HOH:O	2.38	0.50
4:D:85:MET:CE	4:D:96:GLU:HG2	2.66	0.50
1:A:214:MET:CG	27:A:611:PL9:H102	2.29	0.50
26:C:515:BCR:H382	26:C:515:BCR:H23C	1.98	0.50
31:B:622:LMT:C12	29:B:634:LMG:H453	2.42	0.49
4:D:11:GLU:N	36:D:419:EDO:O2	2.44	0.49
12:M:20:VAL:CG2	12:M:20:VAL:HG11	2.77	0.49
2:B:86:ILE:CG1	44:B:909:HOH:O	50.51	0.49
3:C:88:LEU:HD13	24:C:503:CLA:HED3	2.73	0.49
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.94	0.49
16:V:102:PRO:O	16:V:105:ARG:HG3	2.89	0.49
24:B:602:CLA:H93	33:H:106:PG4:C1	2.43	0.49
44:A:756:HOH:O	30:C:528:GOL:C1	2.54	0.49
12:M:16[B]:LEU:HD23	12:M:16[B]:LEU:C	2.31	0.49
14:T:25[A]:GLU:HB2	30:T:101:GOL:H2	2.25	0.49
1:A:230:THR:C	44:B:710:HOH:O	27.00	0.49
3:C:41:ARG:NH1	24:C:511:CLA:HMD1	2.40	0.49
26:B:620:BCR:H383	26:B:620:BCR:H23C	2.03	0.49
13:O:42:ARG:O	13:O:241:ALA:HA	2.18	0.49
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.47	0.48
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.45	0.48
13:O:58:ASN:HA	13:O:59:LYS:HB2	5.60	0.48
27:A:611:PL9:HC2	27:A:611:PL9:H103	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ASP:OD1	2:B:127[B]:ARG:NH2	2.45	0.48
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.48
24:C:501:CLA:HMB1	24:C:501:CLA:HBB1	1.95	0.48
13:O:74[A]:GLU:OE2	44:O:401:HOH:O	2.20	0.48
26:B:619:BCR:HC8	26:B:619:BCR:H331	1.95	0.48
1:A:247:ASN:HB3	2:B:482:ILE:HD11	2.11	0.48
24:B:606:CLA:HBB1	24:B:606:CLA:HHC	1.94	0.48
5:E:10:PHE:HE1	41:E:113:HEM:HBD2	1.79	0.48
33:H:106:PG4:O2	33:H:106:PG4:C5	2.61	0.48
3:C:334:PRO:HA	13:O:153:THR:OG1	2.14	0.48
2:B:86:ILE:HG13	44:B:909:HOH:O	51.09	0.47
1:A:63:ILE:HB	3:C:335:THR:HG21	1.95	0.47
12:M:16[B]:LEU:HD21	12:M:16[B]:LEU:CD1	2.61	0.47
26:T:102:BCR:C38	26:T:102:BCR:C23	2.95	0.47
12:M:16[B]:LEU:CG	12:M:16[B]:LEU:CD1	1.54	0.47
35:T:105:P6G:O19	44:T:201:HOH:O	2.20	0.47
24:B:611:CLA:C15	24:B:611:CLA:H192	2.57	0.47
29:A:613:LMG:C43	29:A:613:LMG:C24	2.93	0.47
12:M:33:GLN:HG3	12:M:33:GLN:CD	2.06	0.47
4:D:13:GLY:HA3	36:D:419:EDO:H21	1.97	0.47
26:T:102:BCR:C38	26:T:102:BCR:H23C	2.37	0.47
4:D:49:LEU:HD13	26:D:406:BCR:C15	2.54	0.47
2:B:285:ASN:HB3	44:B:977:HOH:O	15.26	0.46
2:B:223[A]:GLN:OE1	2:B:227:LYS:HD2	2.15	0.46
1:A:249:VAL:HG12	2:B:491:VAL:HG23	2.25	0.46
26:K:101:BCR:H321	26:K:101:BCR:HC8	1.97	0.46
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.21	0.46
24:B:602:CLA:H143	24:B:602:CLA:C1B	2.44	0.46
31:Y:101:LMT:O2B	31:Y:101:LMT:H4'	2.16	0.46
26:A:610:BCR:H382	26:A:610:BCR:C23	2.46	0.46
24:B:608:CLA:HBB1	24:B:608:CLA:HMB1	2.05	0.46
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.01	0.46
3:C:53:HIS:CB	24:C:512:CLA:HMD1	2.50	0.46
16:V:30:LYS:NZ	44:V:305:HOH:O	2.49	0.46
2:B:24:LEU:HD21	24:B:617:CLA:CAB	2.61	0.46
2:B:223[B]:GLN:NE2	44:B:714:HOH:O	21.60	0.46
13:O:179:GLU:HG2	34:O:308:PGE:O1	40.65	0.45
26:K:101:BCR:C8	26:K:101:BCR:H311	2.46	0.45
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.52	0.45
5:E:9:PRO:HA	32:E:101:LHG:HC2	2.51	0.45
28:A:622:SQD:H382	33:I:104:PG4:H12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:612:SQD:C38	9:J:22:ILE:HD11	2.46	0.45
29:B:634:LMG:H122	29:B:634:LMG:H292	1.98	0.45
3:C:318:LEU:C	3:C:318:LEU:HD23	2.44	0.45
4:D:304:ARG:NH1	44:D:505:HOH:O	2.43	0.45
34:O:308:PGE:H5	44:O:548:HOH:O	2.16	0.45
24:A:607:CLA:HMD3	4:D:182:LEU:HD11	1.98	0.45
27:A:611:PL9:C2	27:A:611:PL9:H103	2.47	0.45
3:C:203:THR:O	3:C:235:GLY:HA3	2.24	0.45
24:C:511:CLA:HBD	24:C:511:CLA:HAA1	1.98	0.45
11:L:9:PRO:HA	31:M:101:LMT:H6D	16.69	0.45
2:B:157:HIS:CE1	24:B:607:CLA:NA	2.85	0.45
2:B:461:LEU:HD22	32:D:409:LHG:H301	1.99	0.44
4:D:272:LEU:C	4:D:272:LEU:HD23	2.42	0.44
5:E:10:PHE:CE1	41:E:113:HEM:HBD2	2.51	0.44
5:E:8[B]:ARG:HB3	5:E:13:ILE:HD11	1.99	0.44
2:B:422:ARG:O	2:B:425:ILE:HG12	2.18	0.44
24:A:606:CLA:CBD	24:D:403:CLA:HAC2	2.47	0.44
24:D:405:CLA:H171	18:X:15[A]:LEU:HG	1.99	0.44
26:B:620:BCR:C23	26:B:620:BCR:H383	2.51	0.44
2:B:237:VAL:HG12	24:B:613:CLA:HMD1	1.99	0.44
38:B:623:HTG:H4	44:O:427:HOH:O	2.16	0.44
24:C:504:CLA:HBB1	24:C:504:CLA:HMB1	1.99	0.44
26:T:102:BCR:H311	26:T:102:BCR:C8	2.44	0.44
25:D:401:PHO:CBB	25:D:401:PHO:HMB1	2.57	0.44
1:A:84:PRO:HA	1:A:112:TYR:CG	2.52	0.44
2:B:84:THR:HG21	44:O:631:HOH:O	86.07	0.44
3:C:391:ARG:NH1	44:C:612:HOH:O	2.50	0.44
26:C:514:BCR:H353	29:C:526:LMG:H262	1.99	0.44
2:B:216:HIS:CE1	24:B:610:CLA:C1A	3.03	0.44
24:C:505:CLA:HBC2	26:C:515:BCR:H341	2.00	0.44
16:V:65:PRO:O	43:V:216:2PE:H242	2.17	0.44
16:V:41:HIS:HA	16:V:45:ILE:O	2.22	0.44
24:B:602:CLA:HHC	24:B:602:CLA:CBB	2.47	0.44
44:C:672:HOH:O	13:O:149:PRO:HB2	13.35	0.43
44:B:926:HOH:O	30:O:305:GOL:C3	75.93	0.43
3:C:149:TYR:CZ	24:C:509:CLA:H201	2.52	0.43
26:D:406:BCR:H341	26:D:406:BCR:H11C	2.09	0.43
13:O:58:ASN:O	13:O:60:ARG:N	2.51	0.43
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.07	0.43
16:V:55[B]:ARG:NH1	44:V:306:HOH:O	2.50	0.43
15:U:51:LYS:HB2	44:U:348:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:607:CLA:CBB	24:B:607:CLA:HMB1	2.40	0.43
3:C:338:GLY:HA3	3:C:341:LEU:O	2.21	0.43
24:C:504:CLA:H142	29:C:519:LMG:C43	2.73	0.43
3:C:57:ALA:HA	44:C:846:HOH:O	43.76	0.43
13:O:66:VAL:HB	13:O:67:PRO:HD2	2.00	0.43
26:K:101:BCR:H331	26:K:101:BCR:HC7	1.98	0.43
26:B:619:BCR:H361	26:B:619:BCR:H20C	1.87	0.43
24:C:507:CLA:H41	24:C:507:CLA:H61	1.83	0.43
4:D:209:LEU:HD23	4:D:209:LEU:C	2.38	0.43
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.58	0.43
25:A:608:PHO:NC	25:A:608:PHO:ND	2.67	0.43
3:C:353:GLY:H	30:C:528:GOL:C2	2.31	0.43
4:D:192:THR:HG23	24:D:404:CLA:HBC2	2.01	0.43
11:L:14:ARG:HB3	14:T:25[A]:GLU:HG2	2.01	0.43
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.88	0.43
3:C:128:GLY:HA3	24:C:513:CLA:C3C	2.49	0.43
24:D:403:CLA:H162	24:D:403:CLA:H203	1.65	0.43
13:O:69:LYS:NZ	44:O:424:HOH:O	18.23	0.43
26:T:102:BCR:H331	26:T:102:BCR:HC7	1.80	0.43
30:U:201:GOL:H12	44:U:366:HOH:O	2.19	0.43
26:A:610:BCR:H382	26:A:610:BCR:H23C	2.01	0.42
24:B:615:CLA:H72	26:B:618:BCR:H362	2.01	0.42
5:E:27:ILE:HG12	41:E:113:HEM:HMC3	2.01	0.42
28:A:612:SQD:H381	9:J:22:ILE:HD11	2.01	0.42
2:B:63:LEU:N	2:B:64:PRO:HD2	2.40	0.42
1:A:121[A]:LEU:HD23	29:A:613:LMG:H202	2.01	0.42
12:M:5:GLN:C	44:M:203:HOH:O	2.57	0.42
26:C:514:BCR:C8	26:C:514:BCR:H331	2.52	0.42
3:C:356:MET:CE	30:C:528:GOL:H12	2.50	0.42
4:D:27:PHE:CD1	32:E:101:LHG:HC12	5.13	0.42
11:L:13:ASN:C	11:L:13:ASN:HD22	2.25	0.42
11:L:13:ASN:ND2	11:L:16:SER:H	2.18	0.42
16:V:55[B]:ARG:CZ	44:V:306:HOH:O	2.68	0.42
24:C:510:CLA:H192	24:C:510:CLA:HBC3	2.06	0.42
29:B:634:LMG:HC91	29:B:634:LMG:H301	2.01	0.42
15:U:45:LEU:HD21	15:U:71:GLN:HB3	2.17	0.42
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.56	0.42
26:K:101:BCR:H382	26:K:101:BCR:H23C	2.11	0.42
28:A:616:SQD:H222	26:T:102:BCR:C32	2.50	0.42
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.02	0.41
2:B:308:LYS:NZ	30:B:629:GOL:H11	29.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.92	0.41
29:C:526:LMG:H202	38:C:532:HTG:H7'1	2.02	0.41
25:D:401:PHO:HHD	25:D:401:PHO:HBC2	2.07	0.41
24:D:405:CLA:H193	18:X:11:PHE:HB3	2.02	0.41
5:E:13:ILE:HG21	41:E:113:HEM:CAD	2.50	0.41
3:C:25:ASN:HD21	3:C:31:SER:HA	1.84	0.41
3:C:449:ARG:NH1	44:C:610:HOH:O	2.50	0.41
26:C:515:BCR:H20C	26:C:515:BCR:H361	2.07	0.41
3:C:391:ARG:NH2	44:C:607:HOH:O	17.11	0.41
29:B:634:LMG:H121	4:D:23:LYS:NZ	2.35	0.41
4:D:283:ALA:O	4:D:287:VAL:HG23	2.21	0.41
13:O:49[A]:THR:CG2	44:O:610:HOH:O	27.84	0.41
13:O:53:LYS:HE3	13:O:65:PHE:CE1	2.86	0.41
7:H:63[B]:LYS:NZ	44:H:201:HOH:O	2.42	0.41
24:B:615:CLA:C10	29:B:621:LMG:C43	2.99	0.41
26:B:618:BCR:H361	26:B:618:BCR:H20C	1.97	0.41
26:B:620:BCR:C38	26:B:620:BCR:C23	3.04	0.41
4:D:316:THR:HG21	44:D:617:HOH:O	34.17	0.41
3:C:38:GLY:HA3	24:C:511:CLA:HMD3	2.11	0.41
26:D:406:BCR:H383	26:D:406:BCR:H23C	2.01	0.41
5:E:20:TRP:CD1	9:J:8:ILE:HD12	2.56	0.41
26:K:101:BCR:HC8	26:K:101:BCR:H311	2.10	0.41
27:A:611:PL9:H251	27:A:611:PL9:H271	1.79	0.41
5:E:18:ARG:NH1	41:E:113:HEM:O2A	2.52	0.41
26:B:620:BCR:HC8	26:B:620:BCR:C33	2.47	0.41
9:J:7[A]:ARG:NH2	44:J:202:HOH:O	2.54	0.41
24:A:606:CLA:H161	24:A:606:CLA:H203	1.78	0.41
24:B:602:CLA:H142	24:B:602:CLA:H112	1.89	0.41
24:B:615:CLA:HMB1	24:B:615:CLA:CBB	2.59	0.41
2:B:26:HIS:HB2	24:B:613:CLA:HMB2	2.08	0.41
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.03	0.41
30:C:523:GOL:C1	16:V:49:ASN:HD22	2.33	0.41
3:C:441:HIS:CE1	24:C:505:CLA:ND	2.94	0.40
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.06	0.40
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.05	0.40
30:U:201:GOL:C1	44:U:366:HOH:O	2.69	0.40
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.02	0.40
3:C:31:SER:HB2	3:C:41:ARG:HG2	2.17	0.40
3:C:213[B]:LEU:HD21	26:C:515:BCR:C20	2.51	0.40
9:J:26:GLY:HA2	31:J:103:LMT:H81	2.03	0.40
13:O:49[A]:THR:OG1	13:O:236:GLN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:622:SQD:H382	33:I:104:PG4:C1	2.51	0.40
2:B:469:HIS:CE1	24:B:612:CLA:NA	2.94	0.40
3:C:444:HIS:CE1	24:C:508:CLA:NA	2.98	0.40
4:D:316:THR:HG23	44:D:501:HOH:O	2.22	0.40
26:T:102:BCR:H11C	26:T:102:BCR:H341	2.17	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:d:408:DGD:O5E	44:v:404:HOH:O[4_456]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/344 (98%)	332 (99%)	3 (1%)	1 (0%)	44	34
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	44	34
2	B	513/506 (101%)	508 (99%)	5 (1%)	0	100	100
2	b	514/506 (102%)	505 (98%)	9 (2%)	0	100	100
3	C	454/458 (99%)	444 (98%)	9 (2%)	1 (0%)	51	41
3	c	460/458 (100%)	446 (97%)	11 (2%)	3 (1%)	25	13
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	82/83 (99%)	82 (100%)	0	0	100	100
5	e	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	29 (97%)	0	1 (3%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	65/65 (100%)	58 (89%)	7 (11%)	0	100	100
7	h	64/65 (98%)	59 (92%)	4 (6%)	1 (2%)	11	3
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	39/40 (98%)	39 (100%)	0	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	34/36 (94%)	34 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	249/245 (102%)	242 (97%)	3 (1%)	4 (2%)	11	3
13	o	248/245 (101%)	239 (96%)	8 (3%)	1 (0%)	38	26
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	97/104 (93%)	95 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	28 (100%)	0	0	100	100
18	X	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
18	x	38/41 (93%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5280/5362 (98%)	5161 (98%)	106 (2%)	13 (0%)	51	41

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	O	59	LYS

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Mol	Chain	Res	Type
3	C	416	SER
3	c	416[A]	SER
3	c	416[B]	SER
13	o	3	ALA
13	O	3	ALA
13	O	4	THR
3	c	19	ASN
7	h	65	LEU
1	A	259	ILE
6	f	15	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/279 (98%)	271 (99%)	2 (1%)	87	87
1	a	273/279 (98%)	272 (100%)	1 (0%)	93	93
2	B	413/404 (102%)	407 (98%)	6 (2%)	70	67
2	b	414/404 (102%)	403 (97%)	11 (3%)	50	42
3	C	357/357 (100%)	354 (99%)	3 (1%)	85	85
3	c	361/357 (101%)	352 (98%)	9 (2%)	53	45
4	D	277/276 (100%)	275 (99%)	2 (1%)	87	87
4	d	278/276 (101%)	276 (99%)	2 (1%)	87	87
5	E	75/72 (104%)	75 (100%)	0	100	100
5	e	74/72 (103%)	73 (99%)	1 (1%)	71	69
6	F	28/38 (74%)	27 (96%)	1 (4%)	40	29
6	f	26/38 (68%)	25 (96%)	1 (4%)	38	27
7	H	56/54 (104%)	53 (95%)	3 (5%)	26	14
7	h	55/54 (102%)	52 (94%)	3 (6%)	25	14
8	I	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	29/28 (104%)	29 (100%)	0	100	100
9	j	27/28 (96%)	26 (96%)	1 (4%)	39	28
10	K	30/30 (100%)	29 (97%)	1 (3%)	43	33
10	k	30/30 (100%)	29 (97%)	1 (3%)	43	33
11	L	36/35 (103%)	34 (94%)	2 (6%)	25	13
11	l	37/35 (106%)	36 (97%)	1 (3%)	50	42
12	M	32/32 (100%)	32 (100%)	0	100	100
12	m	31/32 (97%)	31 (100%)	0	100	100
13	O	212/206 (103%)	208 (98%)	4 (2%)	62	57
13	o	211/206 (102%)	206 (98%)	5 (2%)	54	47
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	27 (100%)	0	100	100
15	U	86/89 (97%)	85 (99%)	1 (1%)	75	75
15	u	84/89 (94%)	83 (99%)	1 (1%)	75	75
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	118 (100%)	0	100	100
17	Y	23/23 (100%)	23 (100%)	0	100	100
17	y	23/23 (100%)	23 (100%)	0	100	100
18	X	34/34 (100%)	33 (97%)	1 (3%)	48	39
18	x	33/34 (97%)	33 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	38	27
19	z	52/52 (100%)	51 (98%)	1 (2%)	62	57
All	All	4381/4376 (100%)	4315 (98%)	66 (2%)	71	67

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	GLU
1	A	238	LYS
2	B	223[A]	GLN
2	B	223[B]	GLN
2	B	246	PHE
2	B	479	PHE

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Mol	Chain	Res	Type
2	B	489	GLU
2	B	492	GLU
3	C	289	PHE
3	C	315	MET
3	C	418	ASN
4	D	12	ARG
4	D	180	ARG
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
10	K	10	LYS
11	L	1	MET
11	L	13	ASN
13	O	57	LYS
13	O	58	ASN
13	O	62	GLU
13	O	118	LEU
15	U	70	ARG
18	X	40	SER
19	Z	6	GLN
19	Z	42	LEU
1	a	244	GLU
2	b	79	SER
2	b	223[A]	GLN
2	b	223[B]	GLN
2	b	246	PHE
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
2	b	489	GLU
2	b	492	GLU
2	b	505	ARG
2	b	506	SER
3	c	16	GLU
3	c	19	ASN
3	c	145[A]	SER
3	c	145[B]	SER
3	c	289	PHE
3	c	355	THR
3	c	418	ASN
3	c	462[A]	GLU

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Mol	Chain	Res	Type
3	c	462[B]	GLU
4	d	180	ARG
4	d	329	MET
5	e	5	THR
6	f	44	GLN
7	h	12[A]	ARG
7	h	12[B]	ARG
7	h	49	TYR
9	j	7	ARG
10	k	10	LYS
11	l	13	ASN
13	o	23	ASP
13	o	58	ASN
13	o	62	GLU
13	o	89	SER
13	o	118	LEU
15	u	70	ARG
19	z	31	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	315	ASN
1	A	338	ASN
2	B	53	ASN
2	B	281	GLN
2	B	331	ASN
3	C	25	ASN
3	C	201	ASN
3	C	373	ASN
4	D	83	ASN
4	D	98	GLN
4	D	332	GLN
6	F	44	GLN
11	L	13	ASN
13	O	82	GLN
13	O	124	ASN
13	O	130	GLN
13	O	147	ASN
16	V	34	GLN
16	V	118	HIS

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Mol	Chain	Res	Type
19	Z	58	ASN
1	a	315	ASN
1	a	338	ASN
2	b	53	ASN
2	b	281	GLN
2	b	331	ASN
2	b	338	GLN
3	c	19	ASN
3	c	201	ASN
3	c	373	ASN
4	d	61	HIS
4	d	83	ASN
4	d	332	GLN
6	f	44	GLN
11	l	13	ASN
13	o	124	ASN
13	o	132	ASN
13	o	147	ASN
18	x	38	GLN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MHS	D	336	4	9,11,12	0.99	0	9,14,16	2.18	4 (44%)
8	FME	I	1	8	9,9,10	0.73	0	7,9,11	1.08	1 (14%)
12	FME	M	1	12	9,9,10	1.44	1 (11%)	7,9,11	1.46	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	T	1[A]	-	9,9,10	0.86	1 (11%)	7,9,11	1.45	2 (28%)
14	FME	T	1[B]	-	9,9,10	0.69	0	7,9,11	1.34	1 (14%)
4	MHS	d	336	4	9,11,12	1.50	1 (11%)	9,14,16	1.88	2 (22%)
8	FME	i	1	8	9,9,10	0.47	0	7,9,11	1.86	2 (28%)
12	FME	m	1[A]	-	9,9,10	0.75	0	7,9,11	1.40	1 (14%)
12	FME	m	1[B]	-	9,9,10	0.96	0	7,9,11	1.94	1 (14%)
14	FME	t	1[A]	-	9,9,10	1.45	1 (11%)	7,9,11	1.11	1 (14%)
14	FME	t	1[B]	-	9,9,10	0.79	0	7,9,11	1.37	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
4	MHS	D	336	4	-	0/4/6/8	0/1/1/1
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1[A]	-	-	0/6/9/11	0/0/0/0
14	FME	T	1[B]	-	-	0/6/9/11	0/0/0/0
4	MHS	d	336	4	-	0/4/6/8	0/1/1/1
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1[A]	-	-	0/6/9/11	0/0/0/0
12	FME	m	1[B]	-	-	0/6/9/11	0/0/0/0
14	FME	t	1[A]	-	-	0/6/9/11	0/0/0/0
14	FME	t	1[B]	-	-	0/6/9/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336	MHS	CG-ND1	-3.07	1.31	1.38
12	M	1	FME	CA-N	-2.94	1.42	1.46
14	T	1[A]	FME	CA-C	2.01	1.52	1.50
14	t	1[A]	FME	CA-C	3.55	1.54	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	O-C-CA	-3.23	117.61	125.15
12	m	1[B]	FME	CB-CG-SD	-3.21	97.90	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CB-CA-C	-2.88	106.90	111.65
12	m	1[A]	FME	O-C-CA	-2.86	118.48	125.15
14	T	1[B]	FME	O-C-CA	-2.70	118.85	125.15
14	T	1[A]	FME	O-C-CA	-2.69	118.89	125.15
4	d	336	MHS	CG-CB-CA	-2.59	109.14	114.12
8	I	1	FME	O-C-CA	-2.55	119.21	125.15
14	t	1[B]	FME	CB-CA-C	-2.48	107.56	111.65
4	D	336	MHS	O-C-CA	-2.23	118.86	125.02
4	D	336	MHS	CB-CA-C	-2.15	107.27	111.41
14	t	1[B]	FME	O-C-CA	-2.14	120.17	125.15
14	t	1[A]	FME	O-C-CA	-2.11	120.24	125.15
4	D	336	MHS	CD2-NE2-CE1	2.10	109.06	105.78
14	T	1[A]	FME	CG-CB-CA	2.25	119.47	112.97
12	M	1	FME	CG-CB-CA	2.78	121.03	112.97
4	d	336	MHS	CM-ND1-CG	4.39	130.28	124.44
4	D	336	MHS	CM-ND1-CG	5.06	131.17	124.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	336	MHS	2	0
12	M	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 447 ligands modelled in this entry, 18 are monoatomic - leaving 429 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	OEX	A	601	1,3,44	0,15,15	0.00	-	0,32,32	0.00	-
23	BCT	A	605	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	A	606	-	56,73,73	1.59	8 (14%)	65,113,113	2.30	16 (24%)
24	CLA	A	607	44	51,68,73	1.39	8 (15%)	59,107,113	2.70	14 (23%)
25	PHO	A	608	-	67,69,69	1.53	11 (16%)	87,99,99	1.77	17 (19%)
24	CLA	A	609	-	56,73,73	1.45	8 (14%)	65,113,113	2.60	17 (26%)
26	BCR	A	610	-	41,41,41	1.21	4 (9%)	56,56,56	1.51	14 (25%)
27	PL9	A	611	-	55,55,55	1.32	7 (12%)	69,69,69	2.08	17 (24%)
28	SQD	A	612	-	53,54,54	1.12	4 (7%)	63,65,65	2.43	16 (25%)
29	LMG	A	613	-	51,51,55	0.96	3 (5%)	59,59,63	1.02	3 (5%)
30	GOL	A	614	-	5,5,5	1.16	0	5,5,5	0.84	0
30	GOL	A	615	-	5,5,5	0.52	0	5,5,5	1.00	0
28	SQD	A	616	-	53,54,54	1.18	4 (7%)	63,65,65	1.64	12 (19%)
31	LMT	A	617	-	36,36,36	1.11	2 (5%)	47,47,47	1.68	9 (19%)
32	LHG	A	618	-	41,41,48	1.21	2 (4%)	42,47,54	1.30	5 (11%)
33	PG4	A	619	-	12,12,12	0.71	0	11,11,11	0.59	0
34	PGE	A	620	-	6,6,9	0.65	0	5,5,8	0.87	0
34	PGE	A	621	-	9,9,9	0.73	0	8,8,8	0.47	0
28	SQD	A	622	-	53,54,54	1.37	4 (7%)	63,65,65	1.66	10 (15%)
35	P6G	A	623	-	18,18,18	0.69	0	17,17,17	0.55	0
35	P6G	A	624	-	18,18,18	0.59	0	17,17,17	0.55	0
36	EDO	A	625	-	3,3,3	0.62	0	2,2,2	0.39	0
24	CLA	B	602	44	56,73,73	1.69	9 (16%)	65,113,113	3.01	25 (38%)
24	CLA	B	603	-	56,73,73	1.69	9 (16%)	65,113,113	2.39	15 (23%)
24	CLA	B	604	-	56,73,73	1.62	10 (17%)	65,113,113	2.64	17 (26%)
24	CLA	B	605	-	56,73,73	1.58	10 (17%)	65,113,113	3.00	25 (38%)
24	CLA	B	606	-	56,73,73	1.67	12 (21%)	65,113,113	3.01	21 (32%)
24	CLA	B	607	-	46,63,73	1.59	9 (19%)	53,101,113	3.00	16 (30%)
24	CLA	B	608	44	56,73,73	1.51	7 (12%)	65,113,113	2.58	17 (26%)
24	CLA	B	609	-	56,73,73	1.42	8 (14%)	65,113,113	2.59	15 (23%)
24	CLA	B	610	-	56,73,73	1.43	8 (14%)	65,113,113	2.95	19 (29%)
24	CLA	B	611	44	56,73,73	1.49	11 (19%)	65,113,113	2.71	24 (36%)
24	CLA	B	612	-	56,73,73	1.64	12 (21%)	65,113,113	2.96	17 (26%)
24	CLA	B	613	-	56,73,73	1.37	8 (14%)	65,113,113	1.99	13 (20%)
24	CLA	B	614	-	56,73,73	1.53	9 (16%)	65,113,113	2.41	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	615	-	46,63,73	1.62	8 (17%)	53,101,113	2.68	19 (35%)
24	CLA	B	616	-	56,73,73	1.41	9 (16%)	65,113,113	2.67	13 (20%)
24	CLA	B	617	-	51,68,73	1.69	12 (23%)	59,107,113	2.70	20 (33%)
26	BCR	B	618	-	41,41,41	0.96	0	56,56,56	1.53	10 (17%)
26	BCR	B	619	-	41,41,41	1.16	4 (9%)	56,56,56	1.43	8 (14%)
26	BCR	B	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.35	7 (12%)
29	LMG	B	621	-	51,51,55	1.08	3 (5%)	59,59,63	1.71	8 (13%)
31	LMT	B	622	-	36,36,36	0.80	1 (2%)	47,47,47	1.49	7 (14%)
38	HTG	B	623	-	19,19,19	0.97	1 (5%)	23,24,24	1.32	2 (8%)
38	HTG	B	624	-	19,19,19	1.00	1 (5%)	23,24,24	2.09	5 (21%)
30	GOL	B	625	-	5,5,5	0.69	0	5,5,5	1.74	2 (40%)
30	GOL	B	626	-	5,5,5	0.84	0	5,5,5	0.65	0
30	GOL	B	627	-	5,5,5	0.66	0	5,5,5	0.84	0
30	GOL	B	628	-	5,5,5	0.76	0	5,5,5	1.58	1 (20%)
30	GOL	B	629	-	5,5,5	0.89	0	5,5,5	0.38	0
38	HTG	B	630	-	19,19,19	1.09	2 (10%)	23,24,24	1.60	7 (30%)
38	HTG	B	631	-	19,19,19	1.08	3 (15%)	23,24,24	1.29	2 (8%)
32	LHG	B	632	-	48,48,48	0.79	2 (4%)	49,54,54	1.31	7 (14%)
30	GOL	B	633	-	5,5,5	1.23	1 (20%)	5,5,5	1.21	0
29	LMG	B	634	-	55,55,55	1.24	3 (5%)	63,63,63	1.46	13 (20%)
30	GOL	B	635	-	5,5,5	0.75	0	5,5,5	1.12	0
33	PG4	B	636	-	12,12,12	0.57	0	11,11,11	0.58	0
33	PG4	B	637	-	12,12,12	0.81	0	11,11,11	0.53	0
33	PG4	B	638	-	12,12,12	0.82	0	11,11,11	0.74	0
33	PG4	B	639	-	12,12,12	0.91	0	11,11,11	0.71	0
33	PG4	B	640	-	12,12,12	0.67	0	11,11,11	0.41	0
33	PG4	B	641	-	12,12,12	0.72	0	11,11,11	0.60	0
33	PG4	B	642	-	12,12,12	0.82	0	11,11,11	0.62	0
33	PG4	B	643	-	12,12,12	0.56	0	11,11,11	0.54	0
34	PGE	B	644	-	9,9,9	0.57	0	8,8,8	0.44	0
34	PGE	B	645	-	9,9,9	0.73	0	8,8,8	0.67	0
34	PGE	B	646	-	9,9,9	0.55	0	8,8,8	0.47	0
34	PGE	B	647	-	9,9,9	0.71	0	8,8,8	0.65	0
34	PGE	B	648	-	9,9,9	0.86	0	8,8,8	0.70	0
34	PGE	B	649	-	9,9,9	0.90	0	8,8,8	0.55	0
34	PGE	B	650	-	9,9,9	0.64	0	8,8,8	0.37	0
35	P6G	B	651	-	18,18,18	0.53	0	17,17,17	0.67	0
35	P6G	B	652	-	18,18,18	0.83	0	17,17,17	1.06	1 (5%)
39	1PE	B	653	-	15,15,15	0.62	0	14,14,14	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	1PE	B	654	-	15,15,15	0.78	0	14,14,14	0.88	0
36	EDO	B	655	-	3,3,3	0.42	0	2,2,2	0.50	0
36	EDO	B	656	-	3,3,3	1.04	0	2,2,2	0.23	0
36	EDO	B	657	-	3,3,3	0.64	0	2,2,2	0.04	0
36	EDO	B	658	-	3,3,3	0.46	0	2,2,2	0.46	0
24	CLA	C	501	-	56,73,73	1.60	10 (17%)	65,113,113	3.00	17 (26%)
24	CLA	C	502	-	56,73,73	1.43	9 (16%)	65,113,113	2.28	18 (27%)
24	CLA	C	503	-	56,73,73	1.69	11 (19%)	65,113,113	2.59	17 (26%)
24	CLA	C	504	44	51,68,73	1.57	12 (23%)	59,107,113	2.52	16 (27%)
24	CLA	C	505	-	56,73,73	1.71	10 (17%)	65,113,113	2.71	15 (23%)
24	CLA	C	506	-	56,73,73	1.61	11 (19%)	65,113,113	2.69	17 (26%)
24	CLA	C	507	44	56,73,73	1.64	11 (19%)	65,113,113	2.81	18 (27%)
24	CLA	C	508	-	51,68,73	1.73	11 (21%)	59,107,113	2.64	16 (27%)
24	CLA	C	509	-	56,73,73	1.44	8 (14%)	65,113,113	2.63	18 (27%)
24	CLA	C	510	-	56,73,73	1.64	11 (19%)	65,113,113	2.44	20 (30%)
24	CLA	C	511	3	56,73,73	1.63	8 (14%)	65,113,113	2.25	18 (27%)
24	CLA	C	512	-	56,73,73	1.62	11 (19%)	65,113,113	2.45	21 (32%)
24	CLA	C	513	-	56,73,73	1.57	8 (14%)	65,113,113	2.67	20 (30%)
26	BCR	C	514	-	41,41,41	1.28	4 (9%)	56,56,56	1.85	13 (23%)
26	BCR	C	515	-	41,41,41	0.96	1 (2%)	56,56,56	1.61	11 (19%)
40	DGD	C	516	-	63,63,67	0.89	5 (7%)	77,77,81	1.33	12 (15%)
40	DGD	C	517	-	57,57,67	0.87	3 (5%)	71,71,81	1.11	2 (2%)
40	DGD	C	518	-	63,63,67	0.78	2 (3%)	77,77,81	1.13	7 (9%)
29	LMG	C	519	-	51,51,55	1.11	3 (5%)	59,59,63	1.58	9 (15%)
29	LMG	C	520	-	51,51,55	1.25	3 (5%)	59,59,63	1.31	9 (15%)
38	HTG	C	521	-	19,19,19	0.91	1 (5%)	23,24,24	1.10	2 (8%)
38	HTG	C	522	-	19,19,19	1.07	1 (5%)	23,24,24	2.11	3 (13%)
30	GOL	C	523	-	5,5,5	0.67	0	5,5,5	2.07	2 (40%)
30	GOL	C	524	-	5,5,5	0.78	0	5,5,5	1.00	0
26	BCR	C	525	-	41,41,41	1.11	3 (7%)	56,56,56	1.67	11 (19%)
29	LMG	C	526	-	55,55,55	1.03	2 (3%)	63,63,63	1.57	9 (14%)
30	GOL	C	527	-	5,5,5	0.44	0	5,5,5	0.28	0
30	GOL	C	528	-	5,5,5	0.70	0	5,5,5	2.93	3 (60%)
38	HTG	C	529	-	19,19,19	1.16	1 (5%)	23,24,24	2.60	4 (17%)
38	HTG	C	530	-	19,19,19	1.02	1 (5%)	23,24,24	1.25	3 (13%)
38	HTG	C	531	-	19,19,19	1.29	1 (5%)	23,24,24	1.06	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	HTG	C	532	-	19,19,19	1.14	2 (10%)	23,24,24	1.77	6 (26%)
31	LMT	C	533	-	36,36,36	0.68	1 (2%)	47,47,47	1.16	3 (6%)
33	PG4	C	534	-	12,12,12	0.73	0	11,11,11	0.40	0
33	PG4	C	535	-	12,12,12	0.96	0	11,11,11	0.81	0
33	PG4	C	536	-	12,12,12	0.70	0	11,11,11	0.65	0
33	PG4	C	537	-	12,12,12	0.67	0	11,11,11	0.57	0
33	PG4	C	538	-	12,12,12	0.77	0	11,11,11	0.55	0
34	PGE	C	539	-	9,9,9	0.93	0	8,8,8	0.84	0
34	PGE	C	540	-	9,9,9	0.61	0	8,8,8	0.32	0
35	P6G	C	541	-	18,18,18	0.66	0	17,17,17	0.43	0
36	EDO	C	542	-	3,3,3	0.51	0	2,2,2	0.39	0
25	PHO	D	401	-	67,69,69	1.78	15 (22%)	87,99,99	1.73	17 (19%)
30	GOL	D	402	-	5,5,5	0.77	0	5,5,5	1.19	1 (20%)
24	CLA	D	403	44	56,73,73	1.78	11 (19%)	65,113,113	2.47	13 (20%)
24	CLA	D	404	-	56,73,73	1.59	13 (23%)	65,113,113	2.68	20 (30%)
24	CLA	D	405	-	56,73,73	1.51	8 (14%)	65,113,113	2.46	16 (24%)
26	BCR	D	406	-	41,41,41	1.41	5 (12%)	56,56,56	1.96	14 (25%)
27	PL9	D	407	-	55,55,55	1.38	7 (12%)	69,69,69	1.33	7 (10%)
40	DGD	D	408	-	67,67,67	1.21	5 (7%)	81,81,81	1.65	11 (13%)
32	LHG	D	409	-	48,48,48	0.83	2 (4%)	49,54,54	1.55	5 (10%)
32	LHG	D	410	-	48,48,48	0.86	2 (4%)	49,54,54	0.99	1 (2%)
32	LHG	D	411	-	48,48,48	0.86	2 (4%)	49,54,54	0.86	3 (6%)
30	GOL	D	412	-	5,5,5	0.58	0	5,5,5	0.64	0
30	GOL	D	413	-	5,5,5	0.53	0	5,5,5	0.80	0
33	PG4	D	414	-	12,12,12	0.67	0	11,11,11	0.50	0
34	PGE	D	415	-	9,9,9	0.60	0	8,8,8	0.41	0
35	P6G	D	416	-	18,18,18	0.72	0	17,17,17	0.59	0
35	P6G	D	417	-	18,18,18	0.65	0	17,17,17	0.87	0
35	P6G	D	418	-	18,18,18	0.75	0	17,17,17	0.59	0
36	EDO	D	419	-	3,3,3	0.69	0	2,2,2	0.08	0
32	LHG	E	101	-	41,41,48	1.09	2 (4%)	42,47,54	1.18	4 (9%)
33	PG4	E	102	-	12,12,12	0.62	0	11,11,11	0.57	0
33	PG4	E	103	-	12,12,12	0.64	0	11,11,11	0.51	0
34	PGE	E	104	-	9,9,9	0.57	0	8,8,8	0.45	0
34	PGE	E	105	-	9,9,9	0.74	0	8,8,8	0.46	0
34	PGE	E	106	-	9,9,9	0.70	0	8,8,8	0.59	0
34	PGE	E	107	-	9,9,9	0.78	0	8,8,8	0.75	0
34	PGE	E	108	-	9,9,9	0.57	0	8,8,8	0.39	0
34	PGE	E	109	-	9,9,9	0.85	0	8,8,8	0.56	0
35	P6G	E	110	-	18,18,18	0.77	0	17,17,17	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	EDO	E	111	-	3,3,3	0.66	0	2,2,2	0.38	0
36	EDO	E	112	-	3,3,3	0.59	0	2,2,2	0.11	0
41	HEM	E	113	5,6	28,50,50	1.29	2 (7%)	17,82,82	3.72	8 (47%)
30	GOL	F	101	42	5,5,5	0.59	0	5,5,5	0.69	0
31	LMT	F	102	-	36,36,36	1.09	3 (8%)	47,47,47	1.29	5 (10%)
28	SQD	F	104	-	53,54,54	1.44	5 (9%)	63,65,65	2.34	17 (26%)
38	HTG	H	101	-	19,19,19	1.09	1 (5%)	23,24,24	1.52	5 (21%)
26	BCR	H	102	-	41,41,41	1.05	3 (7%)	56,56,56	1.76	17 (30%)
40	DGD	H	103	-	63,63,67	1.08	7 (11%)	77,77,81	1.24	12 (15%)
33	PG4	H	104	-	12,12,12	0.63	0	11,11,11	0.34	0
33	PG4	H	105	-	12,12,12	0.75	0	11,11,11	0.47	0
33	PG4	H	106	-	12,12,12	0.74	0	11,11,11	0.62	0
33	PG4	H	107	-	12,12,12	0.71	0	11,11,11	0.49	0
34	PGE	H	108	-	9,9,9	0.61	0	8,8,8	0.59	0
34	PGE	H	109	-	9,9,9	0.53	0	8,8,8	0.48	0
34	PGE	H	110	-	9,9,9	0.57	0	8,8,8	0.33	0
34	PGE	H	111	-	9,9,9	0.67	0	8,8,8	0.38	0
36	EDO	H	112	-	3,3,3	0.49	0	2,2,2	0.38	0
31	LMT	I	101	-	36,36,36	0.89	1 (2%)	47,47,47	1.63	9 (19%)
33	PG4	I	102	-	12,12,12	0.62	0	11,11,11	0.41	0
33	PG4	I	103	-	12,12,12	0.74	0	11,11,11	0.57	0
33	PG4	I	104	-	12,12,12	0.51	0	11,11,11	0.49	0
34	PGE	I	105	-	9,9,9	0.96	0	8,8,8	0.73	0
35	P6G	I	106	-	18,18,18	0.64	0	17,17,17	0.78	1 (5%)
36	EDO	I	107	-	3,3,3	0.73	0	2,2,2	0.17	0
29	LMG	J	101	42	47,47,55	0.73	2 (4%)	55,55,63	0.92	2 (3%)
31	LMT	J	103	-	36,36,36	0.94	1 (2%)	47,47,47	1.63	10 (21%)
33	PG4	J	104	-	12,12,12	0.60	0	11,11,11	0.31	0
33	PG4	J	105	-	12,12,12	0.69	0	11,11,11	0.36	0
34	PGE	J	106	-	9,9,9	0.64	0	8,8,8	0.33	0
34	PGE	J	107	-	9,9,9	0.69	0	8,8,8	0.52	0
34	PGE	J	108	-	9,9,9	0.58	0	8,8,8	0.50	0
36	EDO	J	109	-	3,3,3	0.42	0	2,2,2	0.37	0
26	BCR	K	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.48	11 (19%)
33	PG4	K	102	-	12,12,12	0.63	0	11,11,11	0.49	0
39	1PE	L	101	-	15,15,15	0.68	0	14,14,14	0.65	0
31	LMT	M	101	-	36,36,36	0.97	3 (8%)	47,47,47	1.89	15 (31%)
31	LMT	M	102	-	36,36,36	0.91	0	47,47,47	1.56	2 (4%)
30	GOL	O	302	-	5,5,5	1.49	1 (20%)	5,5,5	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	HTG	O	303	-	19,19,19	1.55	2 (10%)	23,24,24	1.08	2 (8%)
30	GOL	O	304	-	5,5,5	0.40	0	5,5,5	0.48	0
30	GOL	O	305	-	5,5,5	0.43	0	5,5,5	0.34	0
30	GOL	O	306	-	5,5,5	1.26	1 (20%)	5,5,5	1.08	0
30	GOL	O	307	-	5,5,5	0.46	0	5,5,5	0.23	0
34	PGE	O	308	-	9,9,9	1.00	0	8,8,8	1.25	0
34	PGE	O	309	-	9,9,9	0.82	0	8,8,8	0.98	1 (12%)
34	PGE	O	310	-	9,9,9	0.61	0	8,8,8	0.36	0
36	EDO	O	311	-	3,3,3	0.66	0	2,2,2	0.29	0
30	GOL	T	101	-	5,5,5	0.93	0	5,5,5	0.84	0
26	BCR	T	102	-	41,41,41	1.03	4 (9%)	56,56,56	1.62	10 (17%)
30	GOL	T	103	-	5,5,5	0.71	0	5,5,5	0.69	0
34	PGE	T	104	-	6,6,9	1.05	0	5,5,8	0.53	0
35	P6G	T	105	-	18,18,18	0.69	0	17,17,17	0.95	0
30	GOL	U	201	-	5,5,5	0.50	0	5,5,5	1.06	0
33	PG4	U	202	-	12,12,12	0.70	0	11,11,11	0.46	0
30	GOL	V	201	-	5,5,5	1.01	0	5,5,5	0.49	0
41	HEM	V	203	16	28,50,50	1.42	5 (17%)	17,82,82	1.90	5 (29%)
38	HTG	V	204	-	19,19,19	0.94	1 (5%)	23,24,24	2.55	7 (30%)
30	GOL	V	205	-	5,5,5	0.93	0	5,5,5	1.05	0
30	GOL	V	206	-	5,5,5	0.55	0	5,5,5	0.17	0
30	GOL	V	207	-	5,5,5	0.74	0	5,5,5	0.78	0
30	GOL	V	208	-	5,5,5	0.46	0	5,5,5	0.45	0
33	PG4	V	209	-	12,12,12	0.86	0	11,11,11	1.00	1 (9%)
33	PG4	V	210	-	12,12,12	0.91	0	11,11,11	0.77	0
33	PG4	V	211	-	12,12,12	1.03	0	11,11,11	0.80	0
33	PG4	V	212	-	12,12,12	0.72	0	11,11,11	0.55	0
33	PG4	V	213	-	12,12,12	0.71	0	11,11,11	0.62	0
34	PGE	V	214	-	9,9,9	0.64	0	8,8,8	0.30	0
34	PGE	V	215	-	9,9,9	0.87	0	8,8,8	0.62	0
43	2PE	V	216	-	27,27,27	0.92	0	26,26,26	0.68	0
39	1PE	V	217	-	15,15,15	0.95	0	14,14,14	0.98	1 (7%)
36	EDO	V	218	-	3,3,3	0.89	0	2,2,2	0.18	0
33	PG4	X	101	-	12,12,12	0.67	0	11,11,11	0.51	0
33	PG4	X	102	-	12,12,12	0.86	0	11,11,11	0.76	0
33	PG4	X	103	-	12,12,12	0.76	0	11,11,11	0.52	0
36	EDO	X	104	-	3,3,3	0.93	0	2,2,2	0.46	0
31	LMT	Y	101	-	36,36,36	0.59	0	47,47,47	1.32	6 (12%)
34	PGE	Y	102	-	9,9,9	0.80	0	8,8,8	0.60	0
31	LMT	a	401	-	36,36,36	0.83	1 (2%)	47,47,47	1.49	7 (14%)
20	OEX	a	402	1,3,44	0,15,15	0.00	-	0,32,32	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCT	a	406	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	a	407	-	56,73,73	1.45	9 (16%)	65,113,113	2.36	17 (26%)
24	CLA	a	408	44	51,68,73	1.61	10 (19%)	59,107,113	2.82	17 (28%)
25	PHO	a	409	-	67,69,69	1.65	10 (14%)	87,99,99	1.61	18 (20%)
24	CLA	a	410	-	56,73,73	1.53	7 (12%)	65,113,113	2.65	22 (33%)
26	BCR	a	411	-	41,41,41	1.17	3 (7%)	56,56,56	1.33	6 (10%)
27	PL9	a	412	-	55,55,55	1.32	2 (3%)	69,69,69	1.77	15 (21%)
28	SQD	a	413	-	53,54,54	1.13	4 (7%)	63,65,65	2.35	12 (19%)
29	LMG	a	414	-	51,51,55	0.84	2 (3%)	59,59,63	1.27	4 (6%)
30	GOL	a	415	-	5,5,5	1.07	0	5,5,5	1.06	1 (20%)
30	GOL	a	416	-	5,5,5	0.62	0	5,5,5	0.76	0
28	SQD	a	417	-	53,54,54	1.25	4 (7%)	63,65,65	1.45	8 (12%)
38	HTG	a	418	-	19,19,19	1.33	3 (15%)	23,24,24	1.85	8 (34%)
32	LHG	a	419	-	40,40,48	1.20	3 (7%)	41,46,54	1.42	6 (14%)
33	PG4	a	420	-	12,12,12	0.58	0	11,11,11	0.37	0
33	PG4	a	421	-	12,12,12	0.63	0	11,11,11	0.61	0
34	PGE	a	422	-	9,9,9	0.67	0	8,8,8	0.72	0
34	PGE	a	423	-	9,9,9	0.60	0	8,8,8	0.44	0
28	SQD	a	424	-	53,54,54	1.32	4 (7%)	63,65,65	2.24	14 (22%)
36	EDO	a	425	-	3,3,3	0.60	0	2,2,2	0.09	0
24	CLA	b	602	44	56,73,73	1.75	10 (17%)	65,113,113	2.74	24 (36%)
24	CLA	b	603	-	56,73,73	1.63	11 (19%)	65,113,113	2.54	19 (29%)
24	CLA	b	604	-	56,73,73	1.61	11 (19%)	65,113,113	2.51	19 (29%)
24	CLA	b	605	-	56,73,73	1.57	10 (17%)	65,113,113	3.28	22 (33%)
24	CLA	b	606	-	56,73,73	1.76	7 (12%)	65,113,113	2.65	22 (33%)
24	CLA	b	607	-	46,63,73	1.60	9 (19%)	53,101,113	2.72	19 (35%)
24	CLA	b	608	44	56,73,73	1.46	10 (17%)	65,113,113	2.03	12 (18%)
24	CLA	b	609	-	56,73,73	1.53	10 (17%)	65,113,113	2.67	18 (27%)
24	CLA	b	610	-	56,73,73	1.63	10 (17%)	65,113,113	2.80	17 (26%)
24	CLA	b	611	44	56,73,73	1.62	9 (16%)	65,113,113	2.79	23 (35%)
24	CLA	b	612	-	56,73,73	1.43	8 (14%)	65,113,113	2.66	19 (29%)
24	CLA	b	613	-	56,73,73	1.71	11 (19%)	65,113,113	2.64	15 (23%)
24	CLA	b	614	-	56,73,73	1.82	10 (17%)	65,113,113	2.54	16 (24%)
24	CLA	b	615	-	56,73,73	1.49	9 (16%)	65,113,113	2.42	19 (29%)
24	CLA	b	616	-	56,73,73	1.74	8 (14%)	65,113,113	2.58	17 (26%)
24	CLA	b	617	-	51,68,73	1.68	11 (21%)	59,107,113	3.14	20 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	b	618	-	41,41,41	1.12	3 (7%)	56,56,56	1.48	7 (12%)
26	BCR	b	619	-	41,41,41	1.24	5 (12%)	56,56,56	1.76	14 (25%)
26	BCR	b	620	-	41,41,41	0.97	2 (4%)	56,56,56	1.39	4 (7%)
29	LMG	b	621	-	51,51,55	1.02	3 (5%)	59,59,63	1.70	7 (11%)
31	LMT	b	622	-	36,36,36	0.84	1 (2%)	47,47,47	1.47	7 (14%)
38	HTG	b	623	-	19,19,19	1.19	2 (10%)	23,24,24	1.53	5 (21%)
38	HTG	b	624	-	19,19,19	1.49	1 (5%)	23,24,24	1.32	2 (8%)
30	GOL	b	625	-	5,5,5	0.51	0	5,5,5	1.45	1 (20%)
30	GOL	b	626	-	5,5,5	0.78	0	5,5,5	0.74	0
30	GOL	b	627	-	5,5,5	1.23	1 (20%)	5,5,5	1.28	1 (20%)
30	GOL	b	628	-	5,5,5	0.81	0	5,5,5	0.42	0
30	GOL	b	629	-	5,5,5	0.65	0	5,5,5	1.06	0
30	GOL	b	630	-	5,5,5	0.44	0	5,5,5	0.29	0
38	HTG	b	631	-	19,19,19	1.31	2 (10%)	23,24,24	1.66	6 (26%)
38	HTG	b	632	-	19,19,19	0.94	1 (5%)	23,24,24	1.70	7 (30%)
28	SQD	b	633	-	53,54,54	1.43	6 (11%)	63,65,65	2.14	17 (26%)
33	PG4	b	634	-	12,12,12	0.82	0	11,11,11	0.66	0
33	PG4	b	635	-	12,12,12	0.85	0	11,11,11	0.76	0
33	PG4	b	636	-	12,12,12	0.78	0	11,11,11	0.67	0
33	PG4	b	637	-	12,12,12	0.79	0	11,11,11	0.55	0
34	PGE	b	638	-	9,9,9	1.01	0	8,8,8	0.68	0
34	PGE	b	639	-	9,9,9	0.63	0	8,8,8	0.42	0
34	PGE	b	640	-	9,9,9	0.64	0	8,8,8	0.30	0
34	PGE	b	641	-	9,9,9	0.40	0	8,8,8	0.74	0
34	PGE	b	642	-	9,9,9	0.67	0	8,8,8	0.20	0
34	PGE	b	643	-	9,9,9	0.87	0	8,8,8	0.60	0
34	PGE	b	644	-	9,9,9	0.64	0	8,8,8	0.37	0
34	PGE	b	645	-	9,9,9	0.54	0	8,8,8	0.40	0
34	PGE	b	646	-	9,9,9	0.67	0	8,8,8	0.51	0
34	PGE	b	647	-	9,9,9	0.60	0	8,8,8	0.43	0
35	P6G	b	648	-	18,18,18	0.63	0	17,17,17	0.74	0
35	P6G	b	649	-	18,18,18	0.56	0	17,17,17	0.52	0
24	CLA	c	501	-	56,73,73	1.47	8 (14%)	65,113,113	2.74	17 (26%)
24	CLA	c	502	-	56,73,73	1.58	13 (23%)	65,113,113	2.39	14 (21%)
24	CLA	c	503	-	56,73,73	1.50	10 (17%)	65,113,113	2.30	16 (24%)
24	CLA	c	504	44	51,68,73	1.65	11 (21%)	59,107,113	2.77	18 (30%)
24	CLA	c	505	-	56,73,73	1.54	11 (19%)	65,113,113	2.75	17 (26%)
24	CLA	c	506	-	56,73,73	1.53	11 (19%)	65,113,113	2.41	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	507	44	56,73,73	1.70	9 (16%)	65,113,113	2.52	18 (27%)
24	CLA	c	508	-	51,68,73	1.55	9 (17%)	59,107,113	2.77	19 (32%)
24	CLA	c	509	-	56,73,73	1.66	12 (21%)	65,113,113	2.55	17 (26%)
24	CLA	c	510	-	56,73,73	1.84	16 (28%)	65,113,113	2.39	15 (23%)
24	CLA	c	511	3	56,73,73	1.62	13 (23%)	65,113,113	2.56	19 (29%)
24	CLA	c	512	-	56,73,73	1.73	10 (17%)	65,113,113	2.70	19 (29%)
24	CLA	c	513	-	56,73,73	1.69	10 (17%)	65,113,113	2.67	15 (23%)
26	BCR	c	514	-	41,41,41	1.20	5 (12%)	56,56,56	1.69	14 (25%)
26	BCR	c	515	-	41,41,41	1.24	2 (4%)	56,56,56	1.64	12 (21%)
40	DGD	c	516	-	63,63,67	0.90	3 (4%)	77,77,81	1.13	4 (5%)
40	DGD	c	517	-	58,58,67	1.00	4 (6%)	72,72,81	1.15	4 (5%)
40	DGD	c	518	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	7 (9%)
29	LMG	c	519	-	51,51,55	1.00	3 (5%)	59,59,63	1.43	9 (15%)
29	LMG	c	520	-	51,51,55	1.17	3 (5%)	59,59,63	1.22	6 (10%)
31	LMT	c	521	-	36,36,36	0.84	0	47,47,47	1.76	11 (23%)
38	HTG	c	522	-	19,19,19	0.70	0	23,24,24	1.45	4 (17%)
38	HTG	c	523	-	19,19,19	0.91	2 (10%)	23,24,24	1.58	4 (17%)
30	GOL	c	525	-	5,5,5	0.42	0	5,5,5	1.37	1 (20%)
30	GOL	c	526	-	5,5,5	0.36	0	5,5,5	0.81	0
26	BCR	c	527	-	41,41,41	1.02	2 (4%)	56,56,56	1.39	9 (16%)
30	GOL	c	528	-	5,5,5	0.54	0	5,5,5	0.58	0
30	GOL	c	529	-	5,5,5	1.03	0	5,5,5	1.30	0
38	HTG	c	530	-	19,19,19	1.69	3 (15%)	23,24,24	1.32	2 (8%)
38	HTG	c	531	-	19,19,19	1.12	2 (10%)	23,24,24	2.07	6 (26%)
33	PG4	c	532	-	12,12,12	0.91	0	11,11,11	0.78	0
33	PG4	c	533	-	12,12,12	0.59	0	11,11,11	0.47	0
33	PG4	c	534	-	12,12,12	0.55	0	11,11,11	0.43	0
33	PG4	c	535	-	12,12,12	0.86	0	11,11,11	0.67	0
34	PGE	c	536	-	9,9,9	0.62	0	8,8,8	0.27	0
34	PGE	c	537	-	9,9,9	0.55	0	8,8,8	0.35	0
34	PGE	c	538	-	9,9,9	0.92	0	8,8,8	0.87	0
34	PGE	c	539	-	9,9,9	0.65	0	8,8,8	0.36	0
34	PGE	c	540	-	9,9,9	0.68	0	8,8,8	0.45	0
35	P6G	c	541	-	18,18,18	0.51	0	17,17,17	0.42	0
36	EDO	c	542	-	3,3,3	0.62	0	2,2,2	0.41	0
25	PHO	d	401	-	67,69,69	1.57	10 (14%)	87,99,99	1.85	16 (18%)
30	GOL	d	402	-	5,5,5	0.65	0	5,5,5	0.88	0
24	CLA	d	403	44	56,73,73	1.61	9 (16%)	65,113,113	2.09	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	d	404	-	56,73,73	1.43	10 (17%)	65,113,113	2.83	17 (26%)
24	CLA	d	405	-	56,73,73	1.63	10 (17%)	65,113,113	2.46	18 (27%)
26	BCR	d	406	-	41,41,41	1.46	4 (9%)	56,56,56	2.20	16 (28%)
27	PL9	d	407	-	55,55,55	1.23	7 (12%)	69,69,69	1.28	9 (13%)
40	DGD	d	408	-	67,67,67	1.31	4 (5%)	81,81,81	1.77	10 (12%)
32	LHG	d	409	-	48,48,48	0.84	3 (6%)	49,54,54	1.44	6 (12%)
32	LHG	d	410	-	48,48,48	0.79	2 (4%)	49,54,54	1.13	2 (4%)
32	LHG	d	411	-	48,48,48	0.99	3 (6%)	49,54,54	0.85	2 (4%)
29	LMG	d	412	-	55,55,55	1.04	3 (5%)	63,63,63	1.20	5 (7%)
30	GOL	d	413	-	5,5,5	0.76	0	5,5,5	0.90	0
33	PG4	d	414	-	12,12,12	0.73	0	11,11,11	0.44	0
35	P6G	d	415	-	18,18,18	0.70	0	17,17,17	0.93	1 (5%)
35	P6G	d	416	-	18,18,18	0.64	0	17,17,17	0.58	0
36	EDO	d	417	-	3,3,3	0.69	0	2,2,2	0.37	0
32	LHG	e	101	-	41,41,48	1.11	2 (4%)	42,47,54	1.22	4 (9%)
30	GOL	e	102	-	5,5,5	0.67	0	5,5,5	0.77	0
33	PG4	e	103	-	12,12,12	0.59	0	11,11,11	0.49	0
33	PG4	e	104	-	12,12,12	0.61	0	11,11,11	0.55	0
39	1PE	e	105	-	15,15,15	0.65	0	14,14,14	0.53	0
36	EDO	e	106	-	3,3,3	0.41	0	2,2,2	0.52	0
41	HEM	e	107	5,6	28,50,50	1.11	2 (7%)	17,82,82	1.90	4 (23%)
31	LMT	f	101	-	36,36,36	0.94	1 (2%)	47,47,47	1.36	5 (10%)
30	GOL	f	103	42	5,5,5	0.64	0	5,5,5	0.85	0
30	GOL	f	104	-	5,5,5	0.74	0	5,5,5	1.20	0
34	PGE	f	105	-	9,9,9	0.59	0	8,8,8	0.26	0
38	HTG	h	101	-	19,19,19	1.15	2 (10%)	23,24,24	1.68	5 (21%)
26	BCR	h	103	-	41,41,41	1.12	3 (7%)	56,56,56	1.76	16 (28%)
40	DGD	h	104	-	63,63,67	1.11	5 (7%)	77,77,81	1.30	8 (10%)
28	SQD	h	105	-	53,54,54	1.44	6 (11%)	63,65,65	1.77	11 (17%)
33	PG4	h	106	-	12,12,12	0.58	0	11,11,11	0.47	0
34	PGE	h	107	-	9,9,9	0.78	0	8,8,8	0.67	0
34	PGE	h	108	-	9,9,9	0.60	0	8,8,8	0.42	0
34	PGE	h	109	-	9,9,9	0.71	0	8,8,8	0.45	0
34	PGE	h	110	-	9,9,9	0.81	0	8,8,8	0.66	0
33	PG4	i	101	-	12,12,12	0.59	0	11,11,11	0.40	0
33	PG4	i	102	-	12,12,12	0.57	0	11,11,11	0.52	0
33	PG4	i	103	-	12,12,12	0.65	0	11,11,11	0.47	0
33	PG4	i	104	-	12,12,12	0.52	0	11,11,11	0.41	0
34	PGE	i	105	-	9,9,9	0.67	0	8,8,8	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PGE	i	106	-	9,9,9	0.84	0	8,8,8	0.62	0
43	2PE	i	107	-	24,24,27	0.69	0	23,23,26	0.69	0
36	EDO	i	108	-	3,3,3	0.42	0	2,2,2	0.44	0
29	LMG	j	101	42	47,47,55	0.99	3 (6%)	55,55,63	1.07	3 (5%)
31	LMT	j	103	-	36,36,36	0.75	1 (2%)	47,47,47	1.49	7 (14%)
33	PG4	j	104	-	12,12,12	0.71	0	11,11,11	0.71	0
34	PGE	j	105	-	9,9,9	0.65	0	8,8,8	0.58	0
35	P6G	j	106	-	18,18,18	0.81	0	17,17,17	0.74	0
39	1PE	j	107	-	15,15,15	0.63	0	14,14,14	0.62	0
26	BCR	k	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.64	11 (19%)
32	LHG	l	101	-	48,48,48	0.90	2 (4%)	49,54,54	1.21	3 (6%)
28	SQD	l	102	-	53,54,54	1.31	4 (7%)	63,65,65	2.05	15 (23%)
33	PG4	l	103	-	12,12,12	0.66	0	11,11,11	0.49	0
31	LMT	m	101	-	36,36,36	1.04	1 (2%)	47,47,47	1.16	6 (12%)
31	LMT	m	102	-	36,36,36	0.99	1 (2%)	47,47,47	1.70	7 (14%)
30	GOL	m	103	-	5,5,5	0.24	0	5,5,5	0.55	0
23	BCT	m	104[A]	-	0,3,3	0.00	-	0,3,3	0.00	-
23	BCT	m	104[B]	-	0,3,3	0.00	-	0,3,3	0.00	-
38	HTG	o	301	-	19,19,19	1.99	2 (10%)	23,24,24	1.15	1 (4%)
30	GOL	o	303	-	5,5,5	0.74	0	5,5,5	0.64	0
30	GOL	o	304	-	5,5,5	0.47	0	5,5,5	0.82	0
30	GOL	o	305	-	5,5,5	0.68	0	5,5,5	0.90	0
34	PGE	o	306	-	9,9,9	0.61	0	8,8,8	0.24	0
34	PGE	o	307	-	9,9,9	0.79	0	8,8,8	0.54	0
34	PGE	o	308	-	9,9,9	0.69	0	8,8,8	0.55	0
34	PGE	o	309	-	9,9,9	0.85	0	8,8,8	0.70	0
36	EDO	o	310	-	3,3,3	0.61	0	2,2,2	0.10	0
36	EDO	o	311	-	3,3,3	0.47	0	2,2,2	0.30	0
30	GOL	t	101	-	5,5,5	1.24	0	5,5,5	1.09	1 (20%)
26	BCR	t	102	-	41,41,41	1.10	3 (7%)	56,56,56	1.97	18 (32%)
31	LMT	t	103	-	36,36,36	0.86	0	47,47,47	1.46	9 (19%)
34	PGE	t	104	-	9,9,9	0.84	0	8,8,8	0.68	0
34	PGE	t	105	-	6,6,9	0.69	0	5,5,8	0.48	0
30	GOL	u	201	-	5,5,5	0.71	0	5,5,5	1.05	0
30	GOL	u	202	-	5,5,5	0.80	0	5,5,5	0.38	0
31	LMT	u	203	-	36,36,36	1.27	3 (8%)	47,47,47	1.77	9 (19%)
41	HEM	v	202	16	28,50,50	1.36	3 (10%)	17,82,82	1.82	5 (29%)
30	GOL	v	203	-	5,5,5	0.72	0	5,5,5	0.63	0
30	GOL	v	204	-	5,5,5	1.16	0	5,5,5	0.84	0
30	GOL	v	205	-	5,5,5	0.41	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	GOL	v	206	-	5,5,5	0.28	0	5,5,5	0.47	0
30	GOL	v	207	-	5,5,5	0.46	0	5,5,5	0.34	0
28	SQD	x	101	-	53,54,54	1.26	4 (7%)	63,65,65	2.17	15 (23%)
33	PG4	x	102	-	12,12,12	0.65	0	11,11,11	0.36	0
34	PGE	x	103	-	9,9,9	0.61	0	8,8,8	0.56	0
39	1PE	x	104	-	15,15,15	0.63	0	14,14,14	0.41	0
30	GOL	y	101	-	5,5,5	0.63	0	5,5,5	0.67	0
29	LMG	z	101	-	55,55,55	1.02	2 (3%)	63,63,63	1.21	6 (9%)

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
20	OEX	A	601	1,3,44	-	0/0/68/68	0/0/6/6
23	BCT	A	605	21	-	0/0/0/0	0/0/0/0
24	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	607	44	3/3/19/25	0/31/129/135	0/0/9/9
25	PHO	A	608	-	-	0/53/103/103	0/1/6/6
24	CLA	A	609	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	A	610	-	-	0/29/63/63	0/2/2/2
27	PL9	A	611	-	-	0/53/73/73	0/1/1/1
28	SQD	A	612	-	-	0/49/69/69	0/1/1/1
29	LMG	A	613	-	-	0/46/66/70	0/1/1/1
30	GOL	A	614	-	-	0/4/4/4	0/0/0/0
30	GOL	A	615	-	-	0/4/4/4	0/0/0/0
28	SQD	A	616	-	-	0/49/69/69	0/1/1/1
31	LMT	A	617	-	-	0/21/61/61	0/2/2/2
32	LHG	A	618	-	-	0/46/46/53	0/0/0/0
33	PG4	A	619	-	-	0/10/10/10	0/0/0/0
34	PGE	A	620	-	-	0/4/4/7	0/0/0/0
34	PGE	A	621	-	-	0/7/7/7	0/0/0/0
28	SQD	A	622	-	-	0/49/69/69	0/1/1/1
35	P6G	A	623	-	-	0/16/16/16	0/0/0/0
35	P6G	A	624	-	-	0/16/16/16	0/0/0/0
36	EDO	A	625	-	-	0/1/1/1	0/0/0/0
24	CLA	B	602	44	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607	-	3/3/18/25	0/25/123/135	0/0/9/9
24	CLA	B	608	44	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	611	44	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	615	-	3/3/18/25	0/25/123/135	0/0/9/9
24	CLA	B	616	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	617	-	3/3/19/25	0/31/129/135	0/0/9/9
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
29	LMG	B	621	-	-	0/46/66/70	0/1/1/1
31	LMT	B	622	-	-	0/21/61/61	0/2/2/2
38	HTG	B	623	-	-	0/10/30/30	0/1/1/1
38	HTG	B	624	-	-	0/10/30/30	0/1/1/1
30	GOL	B	625	-	-	0/4/4/4	0/0/0/0
30	GOL	B	626	-	-	0/4/4/4	0/0/0/0
30	GOL	B	627	-	-	0/4/4/4	0/0/0/0
30	GOL	B	628	-	-	0/4/4/4	0/0/0/0
30	GOL	B	629	-	-	0/4/4/4	0/0/0/0
38	HTG	B	630	-	-	0/10/30/30	0/1/1/1
38	HTG	B	631	-	-	0/10/30/30	0/1/1/1
32	LHG	B	632	-	-	0/53/53/53	0/0/0/0
30	GOL	B	633	-	-	0/4/4/4	0/0/0/0
29	LMG	B	634	-	-	0/50/70/70	0/1/1/1
30	GOL	B	635	-	-	0/4/4/4	0/0/0/0
33	PG4	B	636	-	-	0/10/10/10	0/0/0/0
33	PG4	B	637	-	-	0/10/10/10	0/0/0/0
33	PG4	B	638	-	-	0/10/10/10	0/0/0/0
33	PG4	B	639	-	-	0/10/10/10	0/0/0/0
33	PG4	B	640	-	-	0/10/10/10	0/0/0/0
33	PG4	B	641	-	-	0/10/10/10	0/0/0/0
33	PG4	B	642	-	-	0/10/10/10	0/0/0/0
33	PG4	B	643	-	-	0/10/10/10	0/0/0/0
34	PGE	B	644	-	-	0/7/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PGE	B	645	-	-	0/7/7/7	0/0/0/0
34	PGE	B	646	-	-	0/7/7/7	0/0/0/0
34	PGE	B	647	-	-	0/7/7/7	0/0/0/0
34	PGE	B	648	-	-	0/7/7/7	0/0/0/0
34	PGE	B	649	-	-	0/7/7/7	0/0/0/0
34	PGE	B	650	-	-	0/7/7/7	0/0/0/0
35	P6G	B	651	-	-	0/16/16/16	0/0/0/0
35	P6G	B	652	-	-	0/16/16/16	0/0/0/0
39	1PE	B	653	-	-	0/13/13/13	0/0/0/0
39	1PE	B	654	-	-	0/13/13/13	0/0/0/0
36	EDO	B	655	-	-	0/1/1/1	0/0/0/0
36	EDO	B	656	-	-	0/1/1/1	0/0/0/0
36	EDO	B	657	-	-	0/1/1/1	0/0/0/0
36	EDO	B	658	-	-	0/1/1/1	0/0/0/0
24	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	44	3/3/19/25	0/31/129/135	0/0/9/9
24	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	507	44	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	508	-	3/3/19/25	0/31/129/135	0/0/9/9
24	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
40	DGD	C	516	-	-	0/51/91/95	0/2/2/2
40	DGD	C	517	-	-	0/45/85/95	0/2/2/2
40	DGD	C	518	-	-	0/51/91/95	0/2/2/2
29	LMG	C	519	-	-	0/46/66/70	0/1/1/1
29	LMG	C	520	-	-	0/46/66/70	0/1/1/1
38	HTG	C	521	-	-	0/10/30/30	0/1/1/1
38	HTG	C	522	-	-	0/10/30/30	0/1/1/1
30	GOL	C	523	-	-	0/4/4/4	0/0/0/0
30	GOL	C	524	-	-	0/4/4/4	0/0/0/0
26	BCR	C	525	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	C	526	-	-	0/50/70/70	0/1/1/1
30	GOL	C	527	-	-	0/4/4/4	0/0/0/0
30	GOL	C	528	-	-	0/4/4/4	0/0/0/0
38	HTG	C	529	-	-	0/10/30/30	0/1/1/1
38	HTG	C	530	-	-	0/10/30/30	0/1/1/1
38	HTG	C	531	-	-	0/10/30/30	0/1/1/1
38	HTG	C	532	-	-	0/10/30/30	0/1/1/1
31	LMT	C	533	-	-	0/21/61/61	0/2/2/2
33	PG4	C	534	-	-	0/10/10/10	0/0/0/0
33	PG4	C	535	-	-	0/10/10/10	0/0/0/0
33	PG4	C	536	-	-	0/10/10/10	0/0/0/0
33	PG4	C	537	-	-	0/10/10/10	0/0/0/0
33	PG4	C	538	-	-	0/10/10/10	0/0/0/0
34	PGE	C	539	-	-	0/7/7/7	0/0/0/0
34	PGE	C	540	-	-	0/7/7/7	0/0/0/0
35	P6G	C	541	-	-	0/16/16/16	0/0/0/0
36	EDO	C	542	-	-	0/1/1/1	0/0/0/0
25	PHO	D	401	-	-	0/53/103/103	0/1/6/6
30	GOL	D	402	-	-	0/4/4/4	0/0/0/0
24	CLA	D	403	44	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	D	405	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	D	406	-	-	0/29/63/63	0/2/2/2
27	PL9	D	407	-	-	0/53/73/73	0/1/1/1
40	DGD	D	408	-	-	2/55/95/95	0/2/2/2
32	LHG	D	409	-	-	0/53/53/53	0/0/0/0
32	LHG	D	410	-	-	0/53/53/53	0/0/0/0
32	LHG	D	411	-	-	0/53/53/53	0/0/0/0
30	GOL	D	412	-	-	0/4/4/4	0/0/0/0
30	GOL	D	413	-	-	0/4/4/4	0/0/0/0
33	PG4	D	414	-	-	0/10/10/10	0/0/0/0
34	PGE	D	415	-	-	0/7/7/7	0/0/0/0
35	P6G	D	416	-	-	0/16/16/16	0/0/0/0
35	P6G	D	417	-	-	0/16/16/16	0/0/0/0
35	P6G	D	418	-	-	0/16/16/16	0/0/0/0
36	EDO	D	419	-	-	0/1/1/1	0/0/0/0
32	LHG	E	101	-	-	0/46/46/53	0/0/0/0
33	PG4	E	102	-	-	0/10/10/10	0/0/0/0
33	PG4	E	103	-	-	0/10/10/10	0/0/0/0
34	PGE	E	104	-	-	0/7/7/7	0/0/0/0
34	PGE	E	105	-	-	0/7/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PGE	E	106	-	-	0/7/7/7	0/0/0/0
34	PGE	E	107	-	-	0/7/7/7	0/0/0/0
34	PGE	E	108	-	-	0/7/7/7	0/0/0/0
34	PGE	E	109	-	-	0/7/7/7	0/0/0/0
35	P6G	E	110	-	-	0/16/16/16	0/0/0/0
36	EDO	E	111	-	-	0/1/1/1	0/0/0/0
36	EDO	E	112	-	-	0/1/1/1	0/0/0/0
41	HEM	E	113	5,6	-	0/6/54/54	0/0/8/8
30	GOL	F	101	42	-	0/4/4/4	0/0/0/0
31	LMT	F	102	-	-	0/21/61/61	0/2/2/2
28	SQD	F	104	-	-	0/49/69/69	0/1/1/1
38	HTG	H	101	-	-	0/10/30/30	0/1/1/1
26	BCR	H	102	-	-	0/29/63/63	0/2/2/2
40	DGD	H	103	-	-	0/51/91/95	0/2/2/2
33	PG4	H	104	-	-	0/10/10/10	0/0/0/0
33	PG4	H	105	-	-	0/10/10/10	0/0/0/0
33	PG4	H	106	-	-	0/10/10/10	0/0/0/0
33	PG4	H	107	-	-	0/10/10/10	0/0/0/0
34	PGE	H	108	-	-	0/7/7/7	0/0/0/0
34	PGE	H	109	-	-	0/7/7/7	0/0/0/0
34	PGE	H	110	-	-	0/7/7/7	0/0/0/0
34	PGE	H	111	-	-	0/7/7/7	0/0/0/0
36	EDO	H	112	-	-	0/1/1/1	0/0/0/0
31	LMT	I	101	-	-	0/21/61/61	0/2/2/2
33	PG4	I	102	-	-	0/10/10/10	0/0/0/0
33	PG4	I	103	-	-	0/10/10/10	0/0/0/0
33	PG4	I	104	-	-	0/10/10/10	0/0/0/0
34	PGE	I	105	-	-	0/7/7/7	0/0/0/0
35	P6G	I	106	-	-	0/16/16/16	0/0/0/0
36	EDO	I	107	-	-	0/1/1/1	0/0/0/0
29	LMG	J	101	42	-	0/42/62/70	0/1/1/1
31	LMT	J	103	-	-	0/21/61/61	0/2/2/2
33	PG4	J	104	-	-	0/10/10/10	0/0/0/0
33	PG4	J	105	-	-	0/10/10/10	0/0/0/0
34	PGE	J	106	-	-	0/7/7/7	0/0/0/0
34	PGE	J	107	-	-	0/7/7/7	0/0/0/0
34	PGE	J	108	-	-	0/7/7/7	0/0/0/0
36	EDO	J	109	-	-	0/1/1/1	0/0/0/0
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
33	PG4	K	102	-	-	0/10/10/10	0/0/0/0
39	1PE	L	101	-	-	0/13/13/13	0/0/0/0
31	LMT	M	101	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
30	GOL	O	302	-	-	0/4/4/4	0/0/0/0
38	HTG	O	303	-	-	0/10/30/30	0/1/1/1
30	GOL	O	304	-	-	0/4/4/4	0/0/0/0
30	GOL	O	305	-	-	0/4/4/4	0/0/0/0
30	GOL	O	306	-	-	0/4/4/4	0/0/0/0
30	GOL	O	307	-	-	0/4/4/4	0/0/0/0
34	PGE	O	308	-	-	0/7/7/7	0/0/0/0
34	PGE	O	309	-	-	0/7/7/7	0/0/0/0
34	PGE	O	310	-	-	0/7/7/7	0/0/0/0
36	EDO	O	311	-	-	0/1/1/1	0/0/0/0
30	GOL	T	101	-	-	0/4/4/4	0/0/0/0
26	BCR	T	102	-	-	0/29/63/63	0/2/2/2
30	GOL	T	103	-	-	0/4/4/4	0/0/0/0
34	PGE	T	104	-	-	0/4/4/7	0/0/0/0
35	P6G	T	105	-	-	0/16/16/16	0/0/0/0
30	GOL	U	201	-	-	0/4/4/4	0/0/0/0
33	PG4	U	202	-	-	0/10/10/10	0/0/0/0
30	GOL	V	201	-	-	0/4/4/4	0/0/0/0
41	HEM	V	203	16	-	0/6/54/54	0/0/8/8
38	HTG	V	204	-	-	0/10/30/30	0/1/1/1
30	GOL	V	205	-	-	0/4/4/4	0/0/0/0
30	GOL	V	206	-	-	0/4/4/4	0/0/0/0
30	GOL	V	207	-	-	0/4/4/4	0/0/0/0
30	GOL	V	208	-	-	0/4/4/4	0/0/0/0
33	PG4	V	209	-	-	0/10/10/10	0/0/0/0
33	PG4	V	210	-	-	0/10/10/10	0/0/0/0
33	PG4	V	211	-	-	0/10/10/10	0/0/0/0
33	PG4	V	212	-	-	0/10/10/10	0/0/0/0
33	PG4	V	213	-	-	0/10/10/10	0/0/0/0
34	PGE	V	214	-	-	0/7/7/7	0/0/0/0
34	PGE	V	215	-	-	0/7/7/7	0/0/0/0
43	2PE	V	216	-	-	0/25/25/25	0/0/0/0
39	1PE	V	217	-	-	0/13/13/13	0/0/0/0
36	EDO	V	218	-	-	0/1/1/1	0/0/0/0
33	PG4	X	101	-	-	0/10/10/10	0/0/0/0
33	PG4	X	102	-	-	0/10/10/10	0/0/0/0
33	PG4	X	103	-	-	0/10/10/10	0/0/0/0
36	EDO	X	104	-	-	0/1/1/1	0/0/0/0
31	LMT	Y	101	-	-	0/21/61/61	0/2/2/2
34	PGE	Y	102	-	-	0/7/7/7	0/0/0/0
31	LMT	a	401	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OEX	a	402	1,3,44	-	0/0/68/68	0/0/6/6
23	BCT	a	406	21	-	0/0/0/0	0/0/0/0
24	CLA	a	407	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	a	408	44	3/3/19/25	0/31/129/135	0/0/9/9
25	PHO	a	409	-	-	0/53/103/103	0/1/6/6
24	CLA	a	410	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	a	411	-	-	0/29/63/63	0/2/2/2
27	PL9	a	412	-	-	0/53/73/73	0/1/1/1
28	SQD	a	413	-	-	0/49/69/69	0/1/1/1
29	LMG	a	414	-	-	0/46/66/70	0/1/1/1
30	GOL	a	415	-	-	0/4/4/4	0/0/0/0
30	GOL	a	416	-	-	0/4/4/4	0/0/0/0
28	SQD	a	417	-	-	0/49/69/69	0/1/1/1
38	HTG	a	418	-	-	0/10/30/30	0/1/1/1
32	LHG	a	419	-	-	0/45/45/53	0/0/0/0
33	PG4	a	420	-	-	0/10/10/10	0/0/0/0
33	PG4	a	421	-	-	0/10/10/10	0/0/0/0
34	PGE	a	422	-	-	0/7/7/7	0/0/0/0
34	PGE	a	423	-	-	0/7/7/7	0/0/0/0
28	SQD	a	424	-	-	0/49/69/69	0/1/1/1
36	EDO	a	425	-	-	0/1/1/1	0/0/0/0
24	CLA	b	602	44	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	607	-	3/3/18/25	0/25/123/135	0/0/9/9
24	CLA	b	608	44	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	611	44	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	616	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	617	-	3/3/19/25	0/31/129/135	0/0/9/9
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
26	BCR	b	620	-	-	0/29/63/63	0/2/2/2
29	LMG	b	621	-	-	0/46/66/70	0/1/1/1
31	LMT	b	622	-	-	0/21/61/61	0/2/2/2
38	HTG	b	623	-	-	0/10/30/30	0/1/1/1
38	HTG	b	624	-	-	0/10/30/30	0/1/1/1
30	GOL	b	625	-	-	0/4/4/4	0/0/0/0
30	GOL	b	626	-	-	0/4/4/4	0/0/0/0
30	GOL	b	627	-	-	0/4/4/4	0/0/0/0
30	GOL	b	628	-	-	0/4/4/4	0/0/0/0
30	GOL	b	629	-	-	0/4/4/4	0/0/0/0
30	GOL	b	630	-	-	0/4/4/4	0/0/0/0
38	HTG	b	631	-	-	0/10/30/30	0/1/1/1
38	HTG	b	632	-	-	0/10/30/30	0/1/1/1
28	SQD	b	633	-	-	0/49/69/69	0/1/1/1
33	PG4	b	634	-	-	0/10/10/10	0/0/0/0
33	PG4	b	635	-	-	0/10/10/10	0/0/0/0
33	PG4	b	636	-	-	0/10/10/10	0/0/0/0
33	PG4	b	637	-	-	0/10/10/10	0/0/0/0
34	PGE	b	638	-	-	0/7/7/7	0/0/0/0
34	PGE	b	639	-	-	0/7/7/7	0/0/0/0
34	PGE	b	640	-	-	0/7/7/7	0/0/0/0
34	PGE	b	641	-	-	0/7/7/7	0/0/0/0
34	PGE	b	642	-	-	0/7/7/7	0/0/0/0
34	PGE	b	643	-	-	0/7/7/7	0/0/0/0
34	PGE	b	644	-	-	0/7/7/7	0/0/0/0
34	PGE	b	645	-	-	0/7/7/7	0/0/0/0
34	PGE	b	646	-	-	0/7/7/7	0/0/0/0
34	PGE	b	647	-	-	0/7/7/7	0/0/0/0
35	P6G	b	648	-	-	0/16/16/16	0/0/0/0
35	P6G	b	649	-	-	0/16/16/16	0/0/0/0
24	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	504	44	3/3/19/25	0/31/129/135	0/0/9/9
24	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	507	44	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	508	-	3/3/19/25	0/31/129/135	0/0/9/9
24	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
26	BCR	c	515	-	-	0/29/63/63	0/2/2/2
40	DGD	c	516	-	-	0/51/91/95	0/2/2/2
40	DGD	c	517	-	-	0/46/86/95	0/2/2/2
40	DGD	c	518	-	-	0/51/91/95	0/2/2/2
29	LMG	c	519	-	-	0/46/66/70	0/1/1/1
29	LMG	c	520	-	-	0/46/66/70	0/1/1/1
31	LMT	c	521	-	-	0/21/61/61	0/2/2/2
38	HTG	c	522	-	-	0/10/30/30	0/1/1/1
38	HTG	c	523	-	-	0/10/30/30	0/1/1/1
30	GOL	c	525	-	-	0/4/4/4	0/0/0/0
30	GOL	c	526	-	-	0/4/4/4	0/0/0/0
26	BCR	c	527	-	-	0/29/63/63	0/2/2/2
30	GOL	c	528	-	-	0/4/4/4	0/0/0/0
30	GOL	c	529	-	-	0/4/4/4	0/0/0/0
38	HTG	c	530	-	-	0/10/30/30	0/1/1/1
38	HTG	c	531	-	-	0/10/30/30	0/1/1/1
33	PG4	c	532	-	-	0/10/10/10	0/0/0/0
33	PG4	c	533	-	-	0/10/10/10	0/0/0/0
33	PG4	c	534	-	-	0/10/10/10	0/0/0/0
33	PG4	c	535	-	-	0/10/10/10	0/0/0/0
34	PGE	c	536	-	-	0/7/7/7	0/0/0/0
34	PGE	c	537	-	-	0/7/7/7	0/0/0/0
34	PGE	c	538	-	-	0/7/7/7	0/0/0/0
34	PGE	c	539	-	-	0/7/7/7	0/0/0/0
34	PGE	c	540	-	-	0/7/7/7	0/0/0/0
35	P6G	c	541	-	-	0/16/16/16	0/0/0/0
36	EDO	c	542	-	-	0/1/1/1	0/0/0/0
25	PHO	d	401	-	-	0/53/103/103	0/1/6/6
30	GOL	d	402	-	-	0/4/4/4	0/0/0/0
24	CLA	d	403	44	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	d	404	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	d	405	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	d	406	-	-	0/29/63/63	0/2/2/2
27	PL9	d	407	-	-	0/53/73/73	0/1/1/1
40	DGD	d	408	-	-	1/55/95/95	0/2/2/2
32	LHG	d	409	-	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	d	410	-	-	0/53/53/53	0/0/0/0
32	LHG	d	411	-	-	0/53/53/53	0/0/0/0
29	LMG	d	412	-	-	1/50/70/70	0/1/1/1
30	GOL	d	413	-	-	0/4/4/4	0/0/0/0
33	PG4	d	414	-	-	0/10/10/10	0/0/0/0
35	P6G	d	415	-	-	0/16/16/16	0/0/0/0
35	P6G	d	416	-	-	0/16/16/16	0/0/0/0
36	EDO	d	417	-	-	0/1/1/1	0/0/0/0
32	LHG	e	101	-	-	0/46/46/53	0/0/0/0
30	GOL	e	102	-	-	0/4/4/4	0/0/0/0
33	PG4	e	103	-	-	0/10/10/10	0/0/0/0
33	PG4	e	104	-	-	0/10/10/10	0/0/0/0
39	1PE	e	105	-	-	0/13/13/13	0/0/0/0
36	EDO	e	106	-	-	0/1/1/1	0/0/0/0
41	HEM	e	107	5,6	-	0/6/54/54	0/0/8/8
31	LMT	f	101	-	-	0/21/61/61	0/2/2/2
30	GOL	f	103	42	-	0/4/4/4	0/0/0/0
30	GOL	f	104	-	-	0/4/4/4	0/0/0/0
34	PGE	f	105	-	-	0/7/7/7	0/0/0/0
38	HTG	h	101	-	-	0/10/30/30	0/1/1/1
26	BCR	h	103	-	-	0/29/63/63	0/2/2/2
40	DGD	h	104	-	-	0/51/91/95	0/2/2/2
28	SQD	h	105	-	-	0/49/69/69	0/1/1/1
33	PG4	h	106	-	-	0/10/10/10	0/0/0/0
34	PGE	h	107	-	-	0/7/7/7	0/0/0/0
34	PGE	h	108	-	-	0/7/7/7	0/0/0/0
34	PGE	h	109	-	-	0/7/7/7	0/0/0/0
34	PGE	h	110	-	-	0/7/7/7	0/0/0/0
33	PG4	i	101	-	-	0/10/10/10	0/0/0/0
33	PG4	i	102	-	-	0/10/10/10	0/0/0/0
33	PG4	i	103	-	-	0/10/10/10	0/0/0/0
33	PG4	i	104	-	-	0/10/10/10	0/0/0/0
34	PGE	i	105	-	-	0/7/7/7	0/0/0/0
34	PGE	i	106	-	-	0/7/7/7	0/0/0/0
43	2PE	i	107	-	-	0/22/22/25	0/0/0/0
36	EDO	i	108	-	-	0/1/1/1	0/0/0/0
29	LMG	j	101	42	-	0/42/62/70	0/1/1/1
31	LMT	j	103	-	-	0/21/61/61	0/2/2/2
33	PG4	j	104	-	-	0/10/10/10	0/0/0/0
34	PGE	j	105	-	-	0/7/7/7	0/0/0/0
35	P6G	j	106	-	-	0/16/16/16	0/0/0/0
39	1PE	j	107	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
32	LHG	l	101	-	-	0/53/53/53	0/0/0/0
28	SQD	l	102	-	-	0/49/69/69	0/1/1/1
33	PG4	l	103	-	-	0/10/10/10	0/0/0/0
31	LMT	m	101	-	-	0/21/61/61	0/2/2/2
31	LMT	m	102	-	-	0/21/61/61	0/2/2/2
30	GOL	m	103	-	-	0/4/4/4	0/0/0/0
23	BCT	m	104[A]	-	-	0/0/0/0	0/0/0/0
23	BCT	m	104[B]	-	-	0/0/0/0	0/0/0/0
38	HTG	o	301	-	-	0/10/30/30	0/1/1/1
30	GOL	o	303	-	-	0/4/4/4	0/0/0/0
30	GOL	o	304	-	-	0/4/4/4	0/0/0/0
30	GOL	o	305	-	-	0/4/4/4	0/0/0/0
34	PGE	o	306	-	-	0/7/7/7	0/0/0/0
34	PGE	o	307	-	-	0/7/7/7	0/0/0/0
34	PGE	o	308	-	-	0/7/7/7	0/0/0/0
34	PGE	o	309	-	-	0/7/7/7	0/0/0/0
36	EDO	o	310	-	-	0/1/1/1	0/0/0/0
36	EDO	o	311	-	-	0/1/1/1	0/0/0/0
30	GOL	t	101	-	-	0/4/4/4	0/0/0/0
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
31	LMT	t	103	-	-	0/21/61/61	0/2/2/2
34	PGE	t	104	-	-	0/7/7/7	0/0/0/0
34	PGE	t	105	-	-	0/4/4/7	0/0/0/0
30	GOL	u	201	-	-	0/4/4/4	0/0/0/0
30	GOL	u	202	-	-	0/4/4/4	0/0/0/0
31	LMT	u	203	-	-	0/21/61/61	0/2/2/2
41	HEM	v	202	16	-	0/6/54/54	0/0/8/8
30	GOL	v	203	-	-	0/4/4/4	0/0/0/0
30	GOL	v	204	-	-	0/4/4/4	0/0/0/0
30	GOL	v	205	-	-	0/4/4/4	0/0/0/0
30	GOL	v	206	-	-	0/4/4/4	0/0/0/0
30	GOL	v	207	-	-	0/4/4/4	0/0/0/0
28	SQD	x	101	-	-	0/49/69/69	0/1/1/1
33	PG4	x	102	-	-	0/10/10/10	0/0/0/0
34	PGE	x	103	-	-	0/7/7/7	0/0/0/0
39	1PE	x	104	-	-	0/13/13/13	0/0/0/0
30	GOL	y	101	-	-	0/4/4/4	0/0/0/0
29	LMG	z	101	-	-	0/50/70/70	0/1/1/1

All (1053) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	o	301	HTG	C1'-S1	-7.79	1.71	1.81
26	d	406	BCR	C30-C25	-5.70	1.46	1.53
38	O	303	HTG	C1'-S1	-5.38	1.74	1.81
26	D	406	BCR	C30-C25	-4.63	1.47	1.53
38	b	624	HTG	C1'-S1	-4.59	1.75	1.81
24	d	403	CLA	C1C-NC	-4.56	1.30	1.37
26	c	515	BCR	C1-C6	-4.53	1.47	1.53
41	E	113	HEM	C1B-NB	-4.47	1.31	1.36
27	D	407	PL9	C36-C37	-4.14	1.39	1.53
38	C	531	HTG	C1'-S1	-3.85	1.76	1.81
24	B	612	CLA	C4C-NC	-3.81	1.31	1.37
41	e	107	HEM	C1B-NB	-3.80	1.32	1.36
27	A	611	PL9	O1-C4	-3.78	1.14	1.23
38	b	631	HTG	C1'-S1	-3.70	1.76	1.81
26	C	514	BCR	C10-C9	-3.58	1.31	1.35
41	V	203	HEM	C1B-NB	-3.56	1.32	1.36
26	D	406	BCR	C1-C6	-3.52	1.49	1.53
38	C	530	HTG	C1'-S1	-3.43	1.77	1.81
27	d	407	PL9	C36-C37	-3.36	1.42	1.53
25	D	401	PHO	C4A-NA	-3.35	1.27	1.35
24	d	405	CLA	C1C-NC	-3.34	1.32	1.37
24	B	617	CLA	C1C-NC	-3.32	1.32	1.37
24	b	613	CLA	CMB-C2B	-3.30	1.44	1.51
38	C	532	HTG	C1'-S1	-3.28	1.77	1.81
26	d	406	BCR	C1-C6	-3.25	1.49	1.53
38	c	530	HTG	C1'-S1	-3.24	1.77	1.81
38	H	101	HTG	C1'-S1	-3.22	1.77	1.81
24	c	506	CLA	C1C-NC	-3.20	1.32	1.37
27	D	407	PL9	C38-C39	-3.20	1.24	1.33
38	C	521	HTG	C1-S1	-3.17	1.75	1.80
24	B	615	CLA	C4C-NC	-3.14	1.32	1.37
28	a	417	SQD	C6-S	-3.11	1.64	1.77
24	c	511	CLA	CMB-C2B	-3.07	1.45	1.51
24	d	405	CLA	CAA-C2A	-3.06	1.48	1.54
25	a	409	PHO	C4A-NA	-3.04	1.27	1.35
24	C	504	CLA	C1C-NC	-3.03	1.32	1.37
29	b	621	LMG	O7-C8	-3.02	1.38	1.46
38	B	624	HTG	C1'-S1	-3.01	1.77	1.81
38	h	101	HTG	C1-S1	-3.01	1.76	1.80
24	B	606	CLA	C1C-NC	-2.97	1.32	1.37
41	v	202	HEM	C1B-NB	-2.92	1.33	1.36
28	A	612	SQD	C6-S	-2.92	1.65	1.77
24	c	505	CLA	C1C-NC	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	a	418	HTG	C1'-S1	-2.84	1.77	1.81
24	b	603	CLA	CHB-C4A	-2.82	1.30	1.33
24	D	404	CLA	CMB-C2B	-2.81	1.45	1.51
38	h	101	HTG	C1'-S1	-2.81	1.77	1.81
26	c	514	BCR	C30-C25	-2.81	1.49	1.53
24	a	408	CLA	C1C-NC	-2.81	1.33	1.37
24	a	407	CLA	CMD-C2D	-2.79	1.45	1.51
24	b	609	CLA	C1C-NC	-2.78	1.33	1.37
24	A	607	CLA	C1C-NC	-2.77	1.33	1.37
27	d	407	PL9	C38-C39	-2.76	1.26	1.33
38	c	531	HTG	C1'-S1	-2.73	1.77	1.81
26	t	102	BCR	C29-C30	-2.72	1.47	1.54
26	c	514	BCR	C1-C6	-2.72	1.50	1.53
26	C	514	BCR	C30-C25	-2.69	1.50	1.53
24	B	611	CLA	C1C-NC	-2.68	1.33	1.37
24	d	404	CLA	CMB-C2B	-2.67	1.46	1.51
38	c	523	HTG	C1'-S1	-2.67	1.78	1.81
24	C	503	CLA	C1C-NC	-2.65	1.33	1.37
24	a	408	CLA	C4C-NC	-2.63	1.33	1.37
24	C	505	CLA	CMD-C2D	-2.63	1.46	1.51
41	E	113	HEM	C4D-ND	-2.62	1.33	1.36
38	C	532	HTG	C1-S1	-2.62	1.76	1.80
24	D	403	CLA	C1C-NC	-2.60	1.33	1.37
24	C	507	CLA	CBD-CGD	-2.60	1.44	1.52
28	A	616	SQD	C6-S	-2.59	1.66	1.77
24	c	502	CLA	C1C-NC	-2.59	1.33	1.37
24	c	510	CLA	CMC-C2C	-2.58	1.45	1.50
24	b	617	CLA	C1C-NC	-2.58	1.33	1.37
24	B	612	CLA	CMD-C2D	-2.58	1.46	1.51
32	d	411	LHG	O8-C6	-2.57	1.39	1.45
24	b	608	CLA	CMB-C2B	-2.57	1.46	1.51
24	c	511	CLA	CMD-C2D	-2.57	1.46	1.51
24	b	610	CLA	CMC-C2C	-2.55	1.45	1.50
41	V	203	HEM	C3B-C2B	-2.53	1.37	1.40
24	B	615	CLA	CHB-C4A	-2.53	1.30	1.33
24	d	404	CLA	C4C-NC	-2.52	1.33	1.37
24	b	614	CLA	CMB-C2B	-2.52	1.46	1.51
25	d	401	PHO	C4A-NA	-2.49	1.29	1.35
24	c	508	CLA	CMD-C2D	-2.49	1.46	1.51
24	b	603	CLA	C4C-NC	-2.49	1.33	1.37
24	C	508	CLA	CMD-C2D	-2.48	1.46	1.51
26	K	101	BCR	C30-C25	-2.46	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	O2D-CED	-2.46	1.39	1.45
25	D	401	PHO	O2A-C1	-2.45	1.38	1.46
28	A	622	SQD	C6-S	-2.44	1.67	1.77
38	B	630	HTG	C1'-S1	-2.44	1.78	1.81
24	c	502	CLA	C4C-NC	-2.44	1.33	1.37
24	b	613	CLA	CMC-C2C	-2.43	1.45	1.50
27	d	407	PL9	C15-C14	-2.42	1.44	1.50
40	C	516	DGD	O5D-C6D	-2.41	1.39	1.43
24	c	501	CLA	C4C-NC	-2.40	1.34	1.37
38	C	522	HTG	C1'-S1	-2.39	1.78	1.81
24	C	503	CLA	O2D-CED	-2.39	1.39	1.45
26	T	102	BCR	C38-C26	-2.38	1.46	1.51
26	d	406	BCR	C32-C1	-2.38	1.48	1.53
38	a	418	HTG	C1-S1	-2.37	1.77	1.80
24	D	403	CLA	C4C-NC	-2.36	1.34	1.37
40	c	518	DGD	O2G-C2G	-2.36	1.40	1.46
26	A	610	BCR	C40-C30	-2.35	1.48	1.53
24	c	510	CLA	CMD-C2D	-2.35	1.46	1.51
29	B	621	LMG	O10-C28	-2.34	1.15	1.22
24	B	616	CLA	C4C-NC	-2.33	1.34	1.37
25	D	401	PHO	C3D-C4D	-2.33	1.36	1.43
24	B	604	CLA	C4-C3	-2.33	1.44	1.50
24	b	605	CLA	O2A-C1	-2.33	1.39	1.46
40	c	517	DGD	O5D-C6D	-2.32	1.39	1.43
26	C	525	BCR	C1-C6	-2.31	1.50	1.53
24	c	502	CLA	O2A-C1	-2.30	1.39	1.46
28	a	413	SQD	C6-S	-2.30	1.68	1.77
26	C	525	BCR	C30-C25	-2.29	1.50	1.53
24	c	511	CLA	C4C-NC	-2.29	1.34	1.37
24	b	611	CLA	O2D-CED	-2.28	1.39	1.45
24	b	604	CLA	C3A-C2A	-2.26	1.48	1.54
25	d	401	PHO	C1D-ND	-2.26	1.33	1.38
28	b	633	SQD	C6-S	-2.25	1.68	1.77
41	e	107	HEM	C4C-NC	-2.25	1.34	1.36
24	C	501	CLA	C1C-NC	-2.25	1.34	1.37
32	d	409	LHG	O7-C5	-2.24	1.40	1.46
29	C	519	LMG	O7-C8	-2.24	1.40	1.46
27	A	611	PL9	C11-C9	-2.23	1.46	1.51
26	h	103	BCR	C21-C22	-2.23	1.32	1.35
25	A	608	PHO	C4A-NA	-2.23	1.29	1.35
27	d	407	PL9	C2-C1	-2.23	1.38	1.44
24	D	405	CLA	C4C-NC	-2.20	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	407	PL9	C51-C49	-2.19	1.44	1.50
24	B	602	CLA	CBD-CGD	-2.19	1.45	1.52
24	a	407	CLA	C4C-NC	-2.19	1.34	1.37
24	c	503	CLA	O2D-CED	-2.18	1.40	1.45
24	c	509	CLA	C1C-NC	-2.17	1.34	1.37
38	B	631	HTG	C1'-S1	-2.17	1.78	1.81
24	b	615	CLA	CMB-C2B	-2.17	1.47	1.51
26	T	102	BCR	C14-C13	-2.17	1.32	1.35
26	k	101	BCR	C30-C25	-2.17	1.50	1.53
24	C	502	CLA	CMD-C2D	-2.17	1.47	1.51
26	b	618	BCR	C40-C30	-2.17	1.49	1.53
24	a	408	CLA	CMB-C2B	-2.16	1.47	1.51
24	d	404	CLA	C1C-NC	-2.16	1.34	1.37
28	x	101	SQD	C6-S	-2.16	1.68	1.77
26	D	406	BCR	C2-C3	-2.14	1.47	1.52
28	h	105	SQD	C6-S	-2.13	1.68	1.77
24	C	501	CLA	CMB-C2B	-2.12	1.47	1.51
40	C	516	DGD	O1G-C1G	-2.12	1.40	1.45
24	B	603	CLA	C1C-NC	-2.11	1.34	1.37
24	c	510	CLA	CMB-C2B	-2.11	1.47	1.51
38	B	631	HTG	C1-S1	-2.11	1.77	1.80
24	C	504	CLA	CMB-C2B	-2.10	1.47	1.51
24	c	510	CLA	CAA-C2A	-2.10	1.50	1.54
24	A	609	CLA	CMB-C2B	-2.10	1.47	1.51
29	c	519	LMG	O7-C8	-2.09	1.41	1.46
24	B	617	CLA	C4C-NC	-2.08	1.34	1.37
24	d	405	CLA	C4C-NC	-2.08	1.34	1.37
24	D	404	CLA	CMD-C2D	-2.08	1.47	1.51
24	a	410	CLA	O2A-C1	-2.07	1.40	1.46
24	B	604	CLA	C1C-NC	-2.07	1.34	1.37
26	b	619	BCR	C30-C25	-2.06	1.51	1.53
24	B	605	CLA	CBD-CGD	-2.06	1.46	1.52
24	B	604	CLA	CMD-C2D	-2.05	1.47	1.51
24	C	504	CLA	CAC-C3C	-2.05	1.45	1.51
25	A	608	PHO	C1C-NC	-2.05	1.34	1.38
26	b	620	BCR	C1-C6	-2.04	1.51	1.53
38	c	523	HTG	C1-S1	-2.04	1.77	1.80
40	C	518	DGD	O2G-C2G	-2.04	1.41	1.46
29	j	101	LMG	O7-C8	-2.03	1.41	1.46
41	V	203	HEM	CAA-C2A	-2.03	1.48	1.52
24	b	608	CLA	CBD-CGD	-2.02	1.46	1.52
32	d	409	LHG	P-O4	-2.02	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	C4C-NC	-2.02	1.34	1.37
24	c	504	CLA	C1C-NC	-2.01	1.34	1.37
24	C	510	CLA	CMC-C2C	-2.01	1.46	1.50
25	D	401	PHO	C1D-ND	-2.00	1.34	1.38
24	B	611	CLA	O2A-CGA	2.00	1.39	1.33
31	u	203	LMT	O5B-C5B	2.00	1.49	1.44
38	B	623	HTG	C1-C2	2.00	1.57	1.53
24	c	505	CLA	C3D-C2D	2.00	1.44	1.39
24	B	611	CLA	CHB-C4A	2.00	1.36	1.33
24	b	604	CLA	C4C-C3C	2.01	1.48	1.45
26	t	102	BCR	C16-C17	2.01	1.49	1.43
24	c	507	CLA	C4B-CHC	2.01	1.45	1.40
26	t	102	BCR	C23-C22	2.01	1.50	1.45
31	j	103	LMT	O1'-C1'	2.01	1.43	1.40
24	D	404	CLA	C3D-C2D	2.01	1.44	1.39
24	c	503	CLA	C4B-CHC	2.01	1.45	1.40
28	F	104	SQD	C4-C5	2.03	1.57	1.53
26	H	102	BCR	C23-C22	2.03	1.50	1.45
24	C	509	CLA	O2D-CGD	2.03	1.38	1.33
26	c	527	BCR	C5-C6	2.03	1.37	1.34
26	B	620	BCR	C15-C14	2.04	1.49	1.43
24	c	502	CLA	C1C-C2C	2.04	1.48	1.44
26	B	619	BCR	C19-C18	2.04	1.50	1.45
38	O	303	HTG	C1-C2	2.04	1.57	1.53
24	d	404	CLA	O2D-CGD	2.05	1.38	1.33
24	c	510	CLA	C1C-C2C	2.05	1.48	1.44
26	b	618	BCR	C12-C13	2.05	1.50	1.45
26	A	610	BCR	C20-C21	2.06	1.49	1.43
24	b	609	CLA	C4B-CHC	2.06	1.45	1.40
31	M	101	LMT	C3B-C2B	2.06	1.57	1.52
24	A	607	CLA	O2A-CGA	2.06	1.39	1.33
26	C	525	BCR	C8-C9	2.07	1.50	1.45
24	c	509	CLA	C4C-C3C	2.07	1.48	1.45
26	b	619	BCR	C19-C18	2.08	1.50	1.45
24	B	613	CLA	O2A-CGA	2.08	1.39	1.33
30	b	627	GOL	O3-C3	2.08	1.51	1.42
24	D	403	CLA	C3B-C2B	2.09	1.43	1.40
40	H	103	DGD	O6D-C1D	2.09	1.47	1.41
24	B	617	CLA	C1C-C2C	2.09	1.48	1.44
24	c	503	CLA	O2A-CGA	2.09	1.39	1.33
24	B	611	CLA	C1B-CHB	2.09	1.45	1.40
26	b	619	BCR	C34-C9	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	514	BCR	C12-C13	2.09	1.50	1.45
32	d	410	LHG	O8-C23	2.10	1.39	1.33
24	c	510	CLA	O2A-CGA	2.10	1.39	1.33
24	B	602	CLA	C2-C3	2.10	1.38	1.33
24	B	616	CLA	C1C-C2C	2.10	1.48	1.44
38	b	623	HTG	O4-C4	2.11	1.47	1.43
24	A	606	CLA	CHB-C4A	2.11	1.36	1.33
40	D	408	DGD	C3G-C2G	2.11	1.56	1.50
24	B	605	CLA	C4B-CHC	2.11	1.45	1.40
24	c	504	CLA	C1C-C2C	2.12	1.48	1.44
27	A	611	PL9	C6-C1	2.12	1.52	1.48
31	C	533	LMT	O1'-C1'	2.12	1.43	1.40
24	b	614	CLA	C4B-CHC	2.12	1.45	1.40
24	a	410	CLA	OBD-CAD	2.12	1.25	1.22
24	C	502	CLA	O2A-CGA	2.12	1.39	1.33
24	C	506	CLA	CHB-C4A	2.12	1.36	1.33
24	c	505	CLA	CHB-C4A	2.13	1.36	1.33
28	F	104	SQD	C3-C2	2.13	1.57	1.52
31	M	101	LMT	O2'-C2'	2.13	1.47	1.43
24	C	501	CLA	O2A-CGA	2.13	1.39	1.33
28	a	424	SQD	C46-C45	2.13	1.56	1.50
24	c	513	CLA	C1C-C2C	2.13	1.48	1.44
24	b	615	CLA	C4B-CHC	2.13	1.45	1.40
26	T	102	BCR	C15-C14	2.13	1.50	1.43
24	b	603	CLA	C4B-CHC	2.14	1.45	1.40
40	H	103	DGD	O6E-C1E	2.14	1.47	1.41
24	b	608	CLA	C4B-CHC	2.14	1.45	1.40
24	B	607	CLA	O2A-CGA	2.15	1.39	1.33
26	h	103	BCR	C19-C18	2.15	1.50	1.45
40	h	104	DGD	O2E-C2E	2.15	1.47	1.43
24	C	504	CLA	CHC-C1C	2.15	1.41	1.35
27	d	407	PL9	C45-C44	2.15	1.56	1.50
40	C	517	DGD	O5D-C1E	2.15	1.43	1.40
26	a	411	BCR	C20-C21	2.15	1.50	1.43
28	b	633	SQD	C46-C45	2.15	1.56	1.50
29	J	101	LMG	O8-C28	2.15	1.39	1.33
24	b	606	CLA	C1C-C2C	2.16	1.48	1.44
24	C	510	CLA	C4C-C3C	2.16	1.48	1.45
24	C	508	CLA	O2D-CGD	2.16	1.38	1.33
24	b	607	CLA	O2A-CGA	2.16	1.39	1.33
24	b	605	CLA	C1C-C2C	2.16	1.48	1.44
24	B	611	CLA	C4B-CHC	2.17	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	632	LHG	O7-C7	2.17	1.40	1.34
26	D	406	BCR	C26-C25	2.17	1.38	1.34
26	c	527	BCR	C8-C9	2.17	1.50	1.45
26	T	102	BCR	C21-C22	2.17	1.38	1.35
26	C	514	BCR	C15-C14	2.17	1.50	1.43
38	b	632	HTG	O5-C1	2.18	1.46	1.42
24	b	610	CLA	C1C-C2C	2.18	1.48	1.44
24	C	506	CLA	C4B-CHC	2.18	1.45	1.40
40	H	103	DGD	O4E-C4E	2.19	1.48	1.43
27	d	407	PL9	C6-C5	2.19	1.46	1.35
24	B	613	CLA	C4B-CHC	2.19	1.46	1.40
24	B	613	CLA	C3D-C2D	2.20	1.44	1.39
29	A	613	LMG	O1-C1	2.20	1.44	1.40
24	A	606	CLA	C1B-CHB	2.20	1.46	1.40
24	B	615	CLA	CBA-CGA	2.20	1.57	1.50
40	h	104	DGD	O4E-C4E	2.21	1.48	1.43
24	c	511	CLA	C4B-CHC	2.21	1.46	1.40
24	B	610	CLA	CHB-C4A	2.21	1.36	1.33
24	c	509	CLA	C4B-CHC	2.22	1.46	1.40
28	b	633	SQD	O6-C1	2.22	1.44	1.40
24	c	510	CLA	CHD-C4C	2.22	1.47	1.41
24	B	604	CLA	C4C-C3C	2.23	1.49	1.45
24	b	617	CLA	C2-C3	2.23	1.38	1.33
24	b	614	CLA	C3B-C2B	2.23	1.43	1.40
24	c	507	CLA	C1C-C2C	2.23	1.48	1.44
24	c	506	CLA	CHD-C4C	2.23	1.47	1.41
24	b	602	CLA	C1C-C2C	2.23	1.48	1.44
24	C	504	CLA	C1B-CHB	2.23	1.46	1.40
38	B	630	HTG	O2-C2	2.24	1.48	1.43
24	B	602	CLA	C4B-CHC	2.24	1.46	1.40
26	C	515	BCR	C12-C13	2.24	1.50	1.45
24	b	608	CLA	O2A-CGA	2.25	1.39	1.33
24	B	612	CLA	O2A-CGA	2.25	1.39	1.33
38	b	631	HTG	O4-C4	2.25	1.48	1.43
32	a	419	LHG	C4-C5	2.25	1.57	1.50
24	C	507	CLA	C4B-CHC	2.25	1.46	1.40
31	u	203	LMT	C1B-C2B	2.25	1.59	1.52
24	C	513	CLA	OBD-CAD	2.26	1.25	1.22
31	J	103	LMT	O1'-C1'	2.26	1.44	1.40
24	A	609	CLA	O2A-CGA	2.26	1.40	1.33
24	c	503	CLA	C3C-C2C	2.26	1.41	1.36
27	A	611	PL9	C48-C49	2.26	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	O	306	GOL	O2-C2	2.27	1.50	1.43
24	C	509	CLA	C1B-CHB	2.27	1.46	1.40
26	d	406	BCR	C8-C9	2.27	1.50	1.45
25	D	401	PHO	CHC-C1C	2.27	1.43	1.38
31	F	102	LMT	C4B-C5B	2.27	1.57	1.53
24	b	612	CLA	OBD-CAD	2.27	1.25	1.22
28	h	105	SQD	C46-C45	2.28	1.57	1.50
25	D	401	PHO	C1C-C2C	2.28	1.50	1.45
26	b	620	BCR	C12-C13	2.28	1.50	1.45
24	B	613	CLA	CHD-C4C	2.28	1.48	1.41
24	b	615	CLA	C3D-C2D	2.28	1.44	1.39
24	C	507	CLA	C1C-C2C	2.28	1.48	1.44
24	c	505	CLA	C1B-CHB	2.29	1.46	1.40
24	C	510	CLA	CHB-C4A	2.29	1.36	1.33
24	c	509	CLA	C1C-C2C	2.30	1.49	1.44
24	B	615	CLA	OBD-CAD	2.30	1.25	1.22
24	C	510	CLA	C1C-C2C	2.30	1.49	1.44
24	C	504	CLA	CHB-C4A	2.30	1.36	1.33
24	c	512	CLA	C4C-C3C	2.30	1.49	1.45
24	c	512	CLA	C4B-CHC	2.31	1.46	1.40
31	F	102	LMT	O4'-C4B	2.31	1.48	1.43
26	B	619	BCR	C35-C13	2.31	1.55	1.50
24	b	604	CLA	CHB-C4A	2.31	1.36	1.33
24	b	607	CLA	C1B-CHB	2.31	1.46	1.40
26	h	103	BCR	C27-C26	2.31	1.55	1.51
24	C	512	CLA	C1C-C2C	2.32	1.49	1.44
30	B	633	GOL	O2-C2	2.32	1.50	1.43
24	C	512	CLA	OBD-CAD	2.33	1.25	1.22
24	B	612	CLA	O2D-CGD	2.33	1.39	1.33
24	D	405	CLA	C4B-CHC	2.33	1.46	1.40
24	C	506	CLA	C1C-C2C	2.33	1.49	1.44
26	b	619	BCR	C5-C6	2.33	1.38	1.34
24	b	604	CLA	C1C-C2C	2.33	1.49	1.44
32	D	409	LHG	C24-C23	2.34	1.57	1.50
24	b	610	CLA	C1B-CHB	2.34	1.46	1.40
38	V	204	HTG	O5-C1	2.34	1.46	1.42
24	b	603	CLA	O2D-CGD	2.35	1.39	1.33
24	B	609	CLA	C4B-CHC	2.35	1.46	1.40
24	c	504	CLA	C3B-C2B	2.35	1.43	1.40
24	B	606	CLA	O1D-CGD	2.36	1.27	1.21
24	b	616	CLA	O2D-CGD	2.36	1.39	1.33
26	H	102	BCR	C12-C13	2.37	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	C2-C3	2.37	1.38	1.33
40	D	408	DGD	O3G-C1D	2.37	1.44	1.40
27	D	407	PL9	O1-C4	2.37	1.28	1.23
24	b	602	CLA	C1B-CHB	2.38	1.46	1.40
31	m	101	LMT	O1'-C1'	2.38	1.44	1.40
24	a	407	CLA	C1B-CHB	2.38	1.46	1.40
40	C	516	DGD	O5D-C1E	2.38	1.44	1.40
32	d	410	LHG	O7-C7	2.39	1.41	1.34
24	a	407	CLA	C4B-CHC	2.39	1.46	1.40
24	B	606	CLA	C1B-CHB	2.39	1.46	1.40
24	B	612	CLA	C1B-CHB	2.39	1.46	1.40
26	b	619	BCR	C24-C25	2.40	1.54	1.45
38	B	631	HTG	O5-C1	2.40	1.46	1.42
24	c	511	CLA	CHD-C4C	2.40	1.48	1.41
25	A	608	PHO	OBD-CAD	2.41	1.26	1.22
24	b	612	CLA	C1C-C2C	2.42	1.49	1.44
38	a	418	HTG	O2-C2	2.42	1.48	1.43
28	l	102	SQD	O5-C1	2.42	1.47	1.41
24	C	507	CLA	O2A-CGA	2.43	1.40	1.33
24	b	612	CLA	O2A-CGA	2.44	1.40	1.33
25	D	401	PHO	O2A-CGA	2.44	1.40	1.33
24	c	502	CLA	C3C-C2C	2.45	1.41	1.36
24	c	506	CLA	C3D-C2D	2.45	1.45	1.39
26	c	515	BCR	C8-C9	2.45	1.51	1.45
24	b	617	CLA	C4B-CHC	2.46	1.46	1.40
24	b	613	CLA	C1B-CHB	2.46	1.46	1.40
26	B	619	BCR	C24-C25	2.46	1.54	1.45
26	A	610	BCR	C23-C22	2.46	1.51	1.45
24	B	603	CLA	C4B-CHC	2.46	1.46	1.40
31	B	622	LMT	O1'-C1'	2.46	1.44	1.40
25	a	409	PHO	OBD-CAD	2.47	1.26	1.22
24	B	606	CLA	CHB-C4A	2.47	1.36	1.33
25	a	409	PHO	O2A-CGA	2.47	1.40	1.33
24	c	508	CLA	C1B-CHB	2.47	1.46	1.40
24	b	616	CLA	CHC-C1C	2.47	1.42	1.35
24	D	404	CLA	C3B-C2B	2.47	1.43	1.40
38	o	301	HTG	C1-C2	2.48	1.57	1.53
38	c	531	HTG	O5-C1	2.48	1.46	1.42
24	B	612	CLA	C3B-C2B	2.49	1.43	1.40
24	C	503	CLA	C4B-CHC	2.49	1.46	1.40
29	a	414	LMG	O8-C28	2.49	1.40	1.33
26	c	514	BCR	C23-C22	2.49	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	607	CLA	C3C-C2C	2.49	1.42	1.36
24	b	611	CLA	O2D-CGD	2.49	1.39	1.33
24	b	604	CLA	O2A-CGA	2.49	1.40	1.33
24	B	614	CLA	C1B-CHB	2.49	1.46	1.40
24	c	502	CLA	C4B-CHC	2.50	1.46	1.40
25	A	608	PHO	CHC-C4B	2.50	1.46	1.40
32	D	411	LHG	O7-C7	2.50	1.41	1.34
25	A	608	PHO	C3D-C2D	2.50	1.45	1.38
31	A	617	LMT	O3B-C3B	2.51	1.48	1.43
24	B	609	CLA	O2D-CGD	2.51	1.39	1.33
24	c	506	CLA	C3B-C2B	2.51	1.43	1.40
38	c	530	HTG	C1-C2	2.51	1.58	1.53
24	b	611	CLA	C4B-CHC	2.51	1.46	1.40
40	H	103	DGD	O2G-C1B	2.51	1.41	1.34
27	A	611	PL9	C2-C3	2.51	1.41	1.34
24	C	505	CLA	C4C-C3C	2.52	1.49	1.45
26	C	514	BCR	C8-C9	2.52	1.51	1.45
24	d	404	CLA	C4B-CHC	2.52	1.46	1.40
24	B	607	CLA	C1C-C2C	2.53	1.49	1.44
40	C	518	DGD	O1G-C1A	2.53	1.40	1.33
32	d	409	LHG	O8-C23	2.53	1.40	1.33
28	h	105	SQD	O6-C1	2.53	1.44	1.40
24	B	614	CLA	CHB-C4A	2.53	1.36	1.33
25	d	401	PHO	C3D-C2D	2.54	1.45	1.38
26	D	406	BCR	C14-C13	2.54	1.39	1.35
24	d	405	CLA	O2D-CGD	2.54	1.39	1.33
29	J	101	LMG	O7-C10	2.54	1.41	1.34
24	C	510	CLA	C1B-CHB	2.55	1.46	1.40
25	d	401	PHO	CHB-C4A	2.55	1.46	1.40
27	D	407	PL9	C6-C5	2.55	1.48	1.35
24	B	615	CLA	C3C-C2C	2.55	1.42	1.36
24	D	404	CLA	C4B-CHC	2.56	1.46	1.40
24	D	403	CLA	O2A-CGA	2.56	1.40	1.33
24	C	502	CLA	OBD-CAD	2.56	1.26	1.22
24	a	410	CLA	O2A-CGA	2.56	1.40	1.33
25	a	409	PHO	O2D-CGD	2.56	1.39	1.33
31	M	101	LMT	O4'-C4B	2.56	1.48	1.43
24	C	502	CLA	C1B-CHB	2.57	1.47	1.40
24	c	513	CLA	C1B-CHB	2.57	1.47	1.40
24	D	404	CLA	C1B-CHB	2.58	1.47	1.40
24	d	404	CLA	C3C-C2C	2.58	1.42	1.36
40	H	103	DGD	O1G-C1A	2.58	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C3B-C2B	2.58	1.43	1.40
24	C	505	CLA	C4B-CHC	2.58	1.47	1.40
28	A	612	SQD	O48-C23	2.58	1.40	1.33
26	B	620	BCR	C23-C22	2.59	1.51	1.45
24	C	512	CLA	C3B-C2B	2.59	1.43	1.40
24	B	616	CLA	C3D-C2D	2.59	1.45	1.39
24	b	605	CLA	OBD-CAD	2.59	1.26	1.22
24	C	508	CLA	C1B-CHB	2.60	1.47	1.40
25	d	401	PHO	CHD-C1D	2.60	1.43	1.38
26	b	618	BCR	C8-C9	2.60	1.51	1.45
24	c	505	CLA	O2A-CGA	2.60	1.41	1.33
26	H	102	BCR	C8-C9	2.60	1.51	1.45
24	b	605	CLA	C3D-C2D	2.60	1.45	1.39
24	c	504	CLA	CHD-C4C	2.60	1.48	1.41
24	a	408	CLA	CHB-C4A	2.61	1.36	1.33
24	B	606	CLA	C3B-C2B	2.61	1.43	1.40
24	B	607	CLA	C3D-C2D	2.62	1.45	1.39
24	c	510	CLA	C1B-CHB	2.62	1.47	1.40
24	B	609	CLA	CHC-C1C	2.63	1.43	1.35
24	B	605	CLA	C3C-C2C	2.64	1.42	1.36
31	a	401	LMT	O1'-C1'	2.64	1.44	1.40
26	a	411	BCR	C8-C9	2.64	1.51	1.45
24	B	614	CLA	O2D-CGD	2.64	1.39	1.33
40	c	516	DGD	O2G-C1B	2.65	1.42	1.34
24	c	509	CLA	C1B-CHB	2.65	1.47	1.40
24	c	511	CLA	C1B-CHB	2.66	1.47	1.40
24	B	612	CLA	C4C-C3C	2.66	1.49	1.45
24	c	503	CLA	C1B-CHB	2.66	1.47	1.40
24	c	507	CLA	C3B-C2B	2.66	1.43	1.40
24	c	501	CLA	OBD-CAD	2.66	1.26	1.22
24	C	503	CLA	C3D-C2D	2.66	1.45	1.39
30	O	302	GOL	O1-C1	2.67	1.53	1.42
24	C	501	CLA	C1C-C2C	2.67	1.49	1.44
24	b	608	CLA	C1B-CHB	2.67	1.47	1.40
24	D	404	CLA	O1D-CGD	2.68	1.28	1.21
24	d	403	CLA	C3D-C2D	2.68	1.45	1.39
24	B	617	CLA	O2A-CGA	2.69	1.41	1.33
24	B	614	CLA	O2A-CGA	2.69	1.41	1.33
24	C	513	CLA	C1B-CHB	2.69	1.47	1.40
31	I	101	LMT	O1'-C1'	2.70	1.44	1.40
24	b	609	CLA	C1B-CHB	2.70	1.47	1.40
24	B	616	CLA	C4C-C3C	2.70	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	404	CLA	O2D-CGD	2.70	1.40	1.33
24	A	607	CLA	C4B-CHC	2.70	1.47	1.40
24	C	503	CLA	C1C-C2C	2.70	1.49	1.44
24	c	506	CLA	OBD-CAD	2.71	1.26	1.22
24	B	617	CLA	C3C-C2C	2.71	1.42	1.36
40	H	103	DGD	O5D-C6D	2.71	1.48	1.43
24	b	608	CLA	O2D-CGD	2.71	1.40	1.33
24	B	613	CLA	O2D-CGD	2.71	1.40	1.33
27	D	407	PL9	C18-C19	2.71	1.39	1.33
40	d	408	DGD	O5D-C1E	2.72	1.44	1.40
24	B	616	CLA	O2A-CGA	2.72	1.41	1.33
24	b	615	CLA	O2D-CGD	2.73	1.40	1.33
32	D	409	LHG	O8-C23	2.73	1.41	1.33
26	A	610	BCR	C21-C22	2.73	1.39	1.35
24	b	605	CLA	O2A-CGA	2.73	1.41	1.33
24	C	506	CLA	C1B-CHB	2.73	1.47	1.40
40	C	517	DGD	O2G-C1B	2.74	1.42	1.34
40	C	516	DGD	O1G-C1A	2.74	1.41	1.33
24	c	505	CLA	O2D-CGD	2.74	1.40	1.33
27	A	611	PL9	C6-C5	2.75	1.49	1.35
24	B	605	CLA	O2D-CGD	2.75	1.40	1.33
31	m	102	LMT	O4'-C4B	2.75	1.49	1.43
24	b	607	CLA	C3D-C2D	2.75	1.45	1.39
24	C	501	CLA	C4B-CHC	2.75	1.47	1.40
26	c	514	BCR	C8-C9	2.75	1.51	1.45
24	c	512	CLA	C1B-CHB	2.75	1.47	1.40
40	c	517	DGD	O5D-C1E	2.75	1.45	1.40
24	B	606	CLA	OBD-CAD	2.76	1.26	1.22
24	B	616	CLA	C3C-C2C	2.76	1.42	1.36
31	A	617	LMT	O1'-C1'	2.76	1.45	1.40
26	a	411	BCR	C36-C18	2.77	1.56	1.50
24	a	408	CLA	O2D-CGD	2.77	1.40	1.33
24	C	504	CLA	C3B-C2B	2.77	1.44	1.40
24	C	502	CLA	C3B-C2B	2.78	1.44	1.40
24	B	605	CLA	C3D-C2D	2.78	1.45	1.39
24	C	508	CLA	O2A-CGA	2.78	1.41	1.33
24	B	609	CLA	OBD-CAD	2.78	1.26	1.22
24	B	606	CLA	C4B-CHC	2.78	1.47	1.40
29	b	621	LMG	O8-C28	2.79	1.41	1.33
24	b	607	CLA	C3C-C2C	2.79	1.42	1.36
24	a	407	CLA	C3D-C2D	2.81	1.45	1.39
24	B	610	CLA	O2A-CGA	2.81	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	412	LMG	O1-C1	2.81	1.45	1.40
24	B	614	CLA	C3B-C2B	2.82	1.44	1.40
24	b	612	CLA	C1B-CHB	2.82	1.47	1.40
38	C	529	HTG	O5-C1	2.82	1.47	1.42
24	b	607	CLA	OBD-CAD	2.82	1.26	1.22
24	b	605	CLA	C1B-CHB	2.82	1.47	1.40
24	C	509	CLA	C3D-C2D	2.82	1.46	1.39
25	d	401	PHO	O2D-CGD	2.83	1.40	1.33
24	b	615	CLA	C3C-C2C	2.83	1.42	1.36
40	c	517	DGD	O2G-C1B	2.83	1.42	1.34
24	b	613	CLA	O2A-CGA	2.84	1.41	1.33
40	H	103	DGD	O5D-C1E	2.84	1.45	1.40
24	B	605	CLA	C1C-C2C	2.84	1.50	1.44
24	C	508	CLA	C1C-C2C	2.84	1.50	1.44
24	C	512	CLA	C1B-CHB	2.84	1.47	1.40
24	b	615	CLA	CHC-C1C	2.85	1.43	1.35
24	b	609	CLA	O2A-CGA	2.85	1.41	1.33
40	D	408	DGD	O5D-C1E	2.85	1.45	1.40
24	c	501	CLA	C1B-CHB	2.85	1.47	1.40
40	c	518	DGD	O2G-C1B	2.85	1.42	1.34
24	D	403	CLA	O2D-CGD	2.86	1.40	1.33
24	C	505	CLA	CHC-C1C	2.86	1.43	1.35
25	D	401	PHO	CHC-C4B	2.86	1.47	1.40
38	b	623	HTG	C1-C2	2.87	1.58	1.53
24	C	504	CLA	O2A-CGA	2.87	1.41	1.33
24	b	610	CLA	C3D-C2D	2.88	1.46	1.39
27	d	407	PL9	C41-C39	2.88	1.57	1.51
27	a	412	PL9	C6-C5	2.88	1.50	1.35
29	j	101	LMG	O8-C28	2.88	1.41	1.33
24	d	403	CLA	C1B-CHB	2.89	1.47	1.40
41	V	203	HEM	CBC-CAC	2.89	1.49	1.28
24	c	511	CLA	CHC-C1C	2.90	1.43	1.35
29	c	520	LMG	O1-C1	2.90	1.45	1.40
24	D	404	CLA	CHC-C1C	2.90	1.43	1.35
32	D	410	LHG	O7-C7	2.90	1.42	1.34
24	d	403	CLA	O2A-CGA	2.90	1.41	1.33
28	a	413	SQD	O48-C23	2.90	1.41	1.33
24	C	512	CLA	C4C-C3C	2.90	1.50	1.45
24	D	404	CLA	C1C-C2C	2.91	1.50	1.44
24	b	606	CLA	C3D-C2D	2.91	1.46	1.39
32	l	101	LHG	O7-C7	2.92	1.42	1.34
24	c	509	CLA	CHC-C1C	2.92	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C3D-C2D	2.92	1.46	1.39
24	B	603	CLA	C3D-C2D	2.92	1.46	1.39
24	C	506	CLA	OBD-CAD	2.92	1.26	1.22
24	c	506	CLA	C1C-C2C	2.93	1.50	1.44
24	B	607	CLA	C1B-CHB	2.93	1.47	1.40
24	B	602	CLA	C3C-C2C	2.93	1.43	1.36
24	C	508	CLA	OBD-CAD	2.93	1.26	1.22
25	a	409	PHO	C3D-C2D	2.94	1.46	1.38
24	b	603	CLA	C1B-CHB	2.94	1.47	1.40
24	D	404	CLA	C3C-C2C	2.95	1.43	1.36
40	C	516	DGD	O2G-C1B	2.95	1.42	1.34
31	b	622	LMT	O3B-C3B	2.95	1.49	1.43
24	b	610	CLA	O2A-CGA	2.95	1.42	1.33
24	b	605	CLA	C3C-C2C	2.95	1.43	1.36
24	b	606	CLA	CHC-C1C	2.96	1.43	1.35
24	c	510	CLA	CHB-C4A	2.96	1.37	1.33
24	c	511	CLA	C3C-C2C	2.96	1.43	1.36
24	C	505	CLA	O2D-CGD	2.97	1.40	1.33
24	c	510	CLA	C4B-CHC	2.97	1.48	1.40
24	A	609	CLA	C4B-CHC	2.98	1.48	1.40
24	B	604	CLA	C3B-C2B	2.98	1.44	1.40
24	b	604	CLA	O2D-CGD	2.98	1.40	1.33
24	c	513	CLA	C4B-CHC	2.98	1.48	1.40
40	c	516	DGD	O5D-C1E	2.98	1.45	1.40
26	B	619	BCR	C17-C18	2.98	1.39	1.35
24	c	504	CLA	O2A-CGA	2.99	1.42	1.33
24	a	407	CLA	CHC-C1C	2.99	1.44	1.35
24	C	506	CLA	O2A-CGA	3.00	1.42	1.33
32	B	632	LHG	O8-C23	3.00	1.42	1.33
24	c	502	CLA	O2A-CGA	3.00	1.42	1.33
24	c	508	CLA	OBD-CAD	3.00	1.26	1.22
24	d	405	CLA	O2A-CGA	3.00	1.42	1.33
24	c	508	CLA	O2D-CGD	3.00	1.40	1.33
24	c	506	CLA	C1B-CHB	3.01	1.48	1.40
24	b	607	CLA	C4B-CHC	3.01	1.48	1.40
24	d	404	CLA	C3B-C2B	3.02	1.44	1.40
24	b	609	CLA	O2D-CGD	3.03	1.40	1.33
24	a	408	CLA	C1B-CHB	3.03	1.48	1.40
24	B	607	CLA	C3B-C2B	3.03	1.44	1.40
24	d	404	CLA	O2A-CGA	3.04	1.42	1.33
24	b	603	CLA	O2A-CGA	3.05	1.42	1.33
24	c	504	CLA	CHC-C1C	3.05	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	520	LMG	O1-C1	3.06	1.45	1.40
24	C	508	CLA	C3D-C2D	3.07	1.46	1.39
24	B	611	CLA	OBD-CAD	3.07	1.26	1.22
25	D	401	PHO	O2D-CGD	3.07	1.41	1.33
24	a	410	CLA	C1B-CHB	3.08	1.48	1.40
24	C	506	CLA	CHC-C1C	3.08	1.44	1.35
24	A	606	CLA	C3B-C2B	3.08	1.44	1.40
24	B	617	CLA	O2D-CGD	3.08	1.41	1.33
24	B	615	CLA	C1B-CHB	3.08	1.48	1.40
32	D	410	LHG	O8-C23	3.08	1.42	1.33
24	c	511	CLA	O2A-CGA	3.09	1.42	1.33
24	b	612	CLA	CHC-C1C	3.09	1.44	1.35
24	c	510	CLA	CHC-C1C	3.10	1.44	1.35
24	a	407	CLA	O2D-CGD	3.10	1.41	1.33
24	C	511	CLA	CHC-C1C	3.10	1.44	1.35
24	C	509	CLA	O2A-CGA	3.10	1.42	1.33
31	f	101	LMT	O1'-C1'	3.11	1.45	1.40
24	b	613	CLA	C4B-CHC	3.11	1.48	1.40
24	b	607	CLA	O2D-CGD	3.11	1.41	1.33
24	B	606	CLA	C3D-C2D	3.11	1.46	1.39
24	B	606	CLA	CHC-C1C	3.11	1.44	1.35
24	D	405	CLA	O2A-CGA	3.12	1.42	1.33
24	b	609	CLA	CHC-C1C	3.12	1.44	1.35
24	c	501	CLA	C3D-C2D	3.12	1.46	1.39
24	C	513	CLA	O2A-CGA	3.13	1.42	1.33
24	c	501	CLA	CHC-C1C	3.13	1.44	1.35
24	C	512	CLA	C3C-C2C	3.13	1.43	1.36
24	b	607	CLA	CHC-C1C	3.13	1.44	1.35
24	c	506	CLA	O2A-CGA	3.14	1.42	1.33
24	b	610	CLA	C3C-C2C	3.14	1.43	1.36
24	B	612	CLA	C3C-C2C	3.15	1.43	1.36
24	d	403	CLA	O2D-CGD	3.15	1.41	1.33
24	b	613	CLA	C3B-C2B	3.15	1.44	1.40
24	b	612	CLA	O2D-CGD	3.16	1.41	1.33
24	C	507	CLA	C1B-CHB	3.16	1.48	1.40
25	A	608	PHO	O2A-CGA	3.16	1.42	1.33
24	b	617	CLA	O2A-CGA	3.16	1.42	1.33
24	B	614	CLA	C3D-C2D	3.17	1.46	1.39
24	B	610	CLA	C3D-C2D	3.17	1.46	1.39
40	C	517	DGD	O1G-C1A	3.17	1.42	1.33
24	C	505	CLA	C3D-C2D	3.17	1.46	1.39
32	D	411	LHG	O8-C23	3.17	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C1B-CHB	3.18	1.48	1.40
24	C	509	CLA	C3C-C2C	3.18	1.43	1.36
29	d	412	LMG	O7-C10	3.18	1.43	1.34
24	c	501	CLA	O2A-CGA	3.18	1.42	1.33
24	C	505	CLA	O2A-CGA	3.19	1.42	1.33
24	B	605	CLA	CHC-C1C	3.19	1.44	1.35
31	F	102	LMT	O1'-C1'	3.19	1.45	1.40
24	b	613	CLA	CHC-C1C	3.19	1.44	1.35
24	B	616	CLA	CHC-C1C	3.19	1.44	1.35
24	B	612	CLA	C3D-C2D	3.20	1.46	1.39
24	b	614	CLA	CHC-C1C	3.21	1.44	1.35
24	b	602	CLA	OBD-CAD	3.21	1.27	1.22
29	b	621	LMG	O7-C10	3.21	1.43	1.34
24	B	608	CLA	C1B-CHB	3.22	1.48	1.40
24	B	608	CLA	OBD-CAD	3.22	1.27	1.22
24	C	509	CLA	CHC-C1C	3.22	1.44	1.35
24	C	504	CLA	O2D-CGD	3.22	1.41	1.33
24	D	405	CLA	C1B-CHB	3.23	1.48	1.40
24	b	614	CLA	C3D-C2D	3.23	1.46	1.39
25	A	608	PHO	C3C-C2C	3.23	1.43	1.36
40	h	104	DGD	O2G-C1B	3.24	1.43	1.34
24	c	505	CLA	C1C-C2C	3.24	1.50	1.44
24	b	610	CLA	C3B-C2B	3.24	1.44	1.40
24	B	617	CLA	C1B-CHB	3.24	1.48	1.40
29	B	621	LMG	O7-C10	3.25	1.43	1.34
28	a	413	SQD	O47-C7	3.25	1.43	1.34
24	c	502	CLA	C1B-CHB	3.25	1.48	1.40
24	d	403	CLA	C3C-C2C	3.26	1.43	1.36
24	b	617	CLA	O2D-CGD	3.26	1.41	1.33
24	C	511	CLA	O2A-CGA	3.26	1.42	1.33
24	b	615	CLA	C1B-CHB	3.26	1.48	1.40
25	A	608	PHO	O2D-CGD	3.27	1.41	1.33
24	c	513	CLA	CHC-C1C	3.27	1.44	1.35
24	c	509	CLA	C3D-C2D	3.27	1.47	1.39
24	B	607	CLA	OBD-CAD	3.27	1.27	1.22
24	B	610	CLA	OBD-CAD	3.27	1.27	1.22
41	V	203	HEM	CBB-CAB	3.27	1.51	1.28
24	c	502	CLA	C3D-C2D	3.28	1.47	1.39
24	B	616	CLA	O2D-CGD	3.28	1.41	1.33
40	c	516	DGD	O1G-C1A	3.29	1.43	1.33
24	c	511	CLA	O2D-CGD	3.29	1.41	1.33
24	C	509	CLA	C3B-C2B	3.29	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	CHC-C1C	3.29	1.44	1.35
24	b	602	CLA	C4B-CHC	3.30	1.48	1.40
24	c	511	CLA	C3B-C2B	3.30	1.44	1.40
24	c	502	CLA	CHC-C1C	3.31	1.44	1.35
24	c	502	CLA	OBD-CAD	3.31	1.27	1.22
24	B	603	CLA	O2D-CGD	3.31	1.41	1.33
24	C	504	CLA	C3C-C2C	3.31	1.43	1.36
24	C	502	CLA	O2D-CGD	3.32	1.41	1.33
24	c	506	CLA	O2D-CGD	3.32	1.41	1.33
24	C	503	CLA	O2A-CGA	3.32	1.43	1.33
24	c	502	CLA	C3B-C2B	3.33	1.44	1.40
24	a	408	CLA	C3C-C2C	3.33	1.43	1.36
24	b	612	CLA	C3C-C2C	3.33	1.43	1.36
24	c	505	CLA	CHC-C1C	3.33	1.45	1.35
29	A	613	LMG	O8-C28	3.33	1.43	1.33
24	B	606	CLA	O2A-CGA	3.33	1.43	1.33
24	B	613	CLA	C3C-C2C	3.34	1.43	1.36
24	c	504	CLA	O2D-CGD	3.34	1.41	1.33
24	d	405	CLA	CHC-C1C	3.34	1.45	1.35
24	b	609	CLA	C3D-C2D	3.34	1.47	1.39
24	C	510	CLA	CHC-C1C	3.35	1.45	1.35
24	b	611	CLA	OBD-CAD	3.35	1.27	1.22
24	b	617	CLA	C3C-C2C	3.36	1.43	1.36
24	B	603	CLA	C1B-CHB	3.36	1.49	1.40
24	d	405	CLA	C3B-C2B	3.36	1.44	1.40
24	c	505	CLA	OBD-CAD	3.37	1.27	1.22
24	b	602	CLA	C3D-C2D	3.37	1.47	1.39
24	A	607	CLA	O2D-CGD	3.37	1.41	1.33
32	d	411	LHG	O8-C23	3.38	1.43	1.33
24	A	606	CLA	C3D-C2D	3.38	1.47	1.39
24	D	403	CLA	C4B-CHC	3.38	1.49	1.40
25	D	401	PHO	C3C-C2C	3.38	1.44	1.36
24	A	607	CLA	C3D-C2D	3.39	1.47	1.39
24	b	617	CLA	C3D-C2D	3.39	1.47	1.39
24	C	512	CLA	O2D-CGD	3.39	1.41	1.33
24	C	504	CLA	C3D-C2D	3.40	1.47	1.39
41	v	202	HEM	CBC-CAC	3.40	1.52	1.28
24	B	609	CLA	O2A-CGA	3.41	1.43	1.33
24	C	506	CLA	C3C-C2C	3.41	1.44	1.36
40	c	518	DGD	O1G-C1A	3.41	1.43	1.33
24	b	602	CLA	C3B-C2B	3.42	1.44	1.40
24	c	508	CLA	CHC-C1C	3.42	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	C3D-C2D	3.43	1.47	1.39
24	c	510	CLA	C3C-C2C	3.43	1.44	1.36
24	b	608	CLA	C3B-C2B	3.44	1.44	1.40
24	c	513	CLA	O2A-CGA	3.45	1.43	1.33
24	B	611	CLA	O2D-CGD	3.45	1.41	1.33
24	c	512	CLA	O2A-CGA	3.45	1.43	1.33
24	C	507	CLA	CHC-C1C	3.45	1.45	1.35
24	c	506	CLA	CHC-C1C	3.46	1.45	1.35
24	A	609	CLA	C3D-C2D	3.46	1.47	1.39
24	B	605	CLA	O2A-CGA	3.46	1.43	1.33
24	b	616	CLA	O2A-CGA	3.47	1.43	1.33
24	B	611	CLA	CHC-C1C	3.47	1.45	1.35
24	c	509	CLA	O2A-CGA	3.47	1.43	1.33
24	b	602	CLA	CHC-C1C	3.47	1.45	1.35
24	b	603	CLA	C3D-C2D	3.47	1.47	1.39
24	B	608	CLA	O2D-CGD	3.47	1.42	1.33
24	A	606	CLA	CHC-C1C	3.47	1.45	1.35
29	a	414	LMG	O7-C10	3.49	1.44	1.34
24	c	503	CLA	OBD-CAD	3.49	1.27	1.22
24	a	408	CLA	CHC-C1C	3.49	1.45	1.35
31	u	203	LMT	O1'-C1'	3.49	1.46	1.40
24	c	504	CLA	CHB-C4A	3.50	1.38	1.33
29	c	519	LMG	O7-C10	3.50	1.44	1.34
24	C	513	CLA	O2D-CGD	3.50	1.42	1.33
24	C	512	CLA	CHB-C4A	3.50	1.38	1.33
24	B	610	CLA	CHC-C1C	3.51	1.45	1.35
24	b	609	CLA	C3B-C2B	3.51	1.45	1.40
24	A	609	CLA	CHC-C1C	3.51	1.45	1.35
24	D	403	CLA	CHC-C1C	3.52	1.45	1.35
24	B	610	CLA	O2D-CGD	3.52	1.42	1.33
40	c	517	DGD	O1G-C1A	3.52	1.43	1.33
24	b	613	CLA	C3C-C2C	3.52	1.44	1.36
24	B	602	CLA	O2D-CGD	3.52	1.42	1.33
24	B	602	CLA	CHC-C1C	3.53	1.45	1.35
24	d	404	CLA	C3D-C2D	3.54	1.47	1.39
24	c	510	CLA	O2D-CGD	3.55	1.42	1.33
24	D	405	CLA	O2D-CGD	3.55	1.42	1.33
25	D	401	PHO	C3D-C2D	3.55	1.48	1.38
24	b	611	CLA	C3D-C2D	3.55	1.47	1.39
24	A	606	CLA	O2D-CGD	3.56	1.42	1.33
24	B	604	CLA	CHC-C1C	3.56	1.45	1.35
27	D	407	PL9	C41-C39	3.56	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	CHC-C1C	3.56	1.45	1.35
24	b	604	CLA	C3D-C2D	3.56	1.47	1.39
24	A	609	CLA	C1B-CHB	3.56	1.49	1.40
25	a	409	PHO	CHC-C1C	3.57	1.45	1.38
24	B	612	CLA	OBD-CAD	3.57	1.27	1.22
40	d	408	DGD	O3G-C1D	3.57	1.46	1.40
24	c	504	CLA	OBD-CAD	3.57	1.27	1.22
24	a	410	CLA	C3C-C2C	3.58	1.44	1.36
25	D	401	PHO	OBD-CAD	3.58	1.28	1.22
32	l	101	LHG	O8-C23	3.58	1.43	1.33
24	b	617	CLA	C1B-CHB	3.58	1.49	1.40
24	B	603	CLA	C3B-C2B	3.60	1.45	1.40
24	C	513	CLA	C3D-C2D	3.60	1.47	1.39
24	B	605	CLA	OBD-CAD	3.60	1.27	1.22
24	c	511	CLA	C3D-C2D	3.60	1.47	1.39
24	C	510	CLA	C3D-C2D	3.60	1.47	1.39
24	b	609	CLA	OBD-CAD	3.60	1.27	1.22
24	B	608	CLA	C3D-C2D	3.61	1.47	1.39
28	l	102	SQD	O47-C7	3.61	1.44	1.34
24	C	511	CLA	O2D-CGD	3.62	1.42	1.33
24	A	609	CLA	OBD-CAD	3.62	1.27	1.22
24	B	608	CLA	CHC-C1C	3.62	1.45	1.35
24	D	404	CLA	OBD-CAD	3.63	1.27	1.22
24	C	501	CLA	CHC-C1C	3.63	1.45	1.35
40	h	104	DGD	O1G-C1A	3.63	1.44	1.33
24	b	608	CLA	CHC-C1C	3.64	1.45	1.35
24	D	403	CLA	CHB-C4A	3.64	1.38	1.33
24	A	609	CLA	C3C-C2C	3.64	1.44	1.36
24	a	408	CLA	C3D-C2D	3.65	1.47	1.39
24	A	607	CLA	OBD-CAD	3.65	1.27	1.22
24	C	502	CLA	C3D-C2D	3.65	1.47	1.39
24	C	506	CLA	C3D-C2D	3.65	1.47	1.39
24	b	603	CLA	C3C-C2C	3.65	1.44	1.36
24	C	507	CLA	OBD-CAD	3.66	1.27	1.22
24	b	606	CLA	O2A-CGA	3.66	1.44	1.33
24	c	509	CLA	O2D-CGD	3.67	1.42	1.33
24	b	611	CLA	CHB-C4A	3.68	1.38	1.33
24	c	508	CLA	O2A-CGA	3.68	1.44	1.33
24	B	608	CLA	C3C-C2C	3.68	1.44	1.36
25	d	401	PHO	OBD-CAD	3.69	1.28	1.22
24	C	505	CLA	C3B-C2B	3.70	1.45	1.40
24	B	610	CLA	C3C-C2C	3.70	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	608	PHO	CHB-C1B	3.70	1.46	1.38
24	B	617	CLA	C3D-C2D	3.71	1.47	1.39
24	C	513	CLA	C3C-C2C	3.71	1.44	1.36
24	C	511	CLA	OBD-CAD	3.71	1.27	1.22
24	c	501	CLA	C3C-C2C	3.72	1.44	1.36
24	b	614	CLA	O2A-CGA	3.72	1.44	1.33
24	b	602	CLA	C3C-C2C	3.72	1.44	1.36
41	v	202	HEM	CBB-CAB	3.73	1.55	1.28
24	b	613	CLA	O2D-CGD	3.73	1.42	1.33
32	d	411	LHG	O7-C7	3.74	1.45	1.34
29	C	519	LMG	O7-C10	3.74	1.45	1.34
24	c	506	CLA	C3C-C2C	3.74	1.44	1.36
24	b	611	CLA	CHC-C1C	3.74	1.46	1.35
24	c	508	CLA	C3D-C2D	3.74	1.48	1.39
24	B	609	CLA	C3D-C2D	3.75	1.48	1.39
29	B	634	LMG	O1-C1	3.75	1.46	1.40
24	B	604	CLA	O2A-CGA	3.76	1.44	1.33
28	A	612	SQD	O47-C7	3.77	1.45	1.34
24	a	410	CLA	C3D-C2D	3.78	1.48	1.39
24	c	509	CLA	C3C-C2C	3.78	1.44	1.36
24	b	605	CLA	O2D-CGD	3.79	1.42	1.33
29	C	526	LMG	O8-C28	3.79	1.44	1.33
25	a	409	PHO	C3C-C2C	3.79	1.44	1.36
24	B	615	CLA	O2A-CGA	3.80	1.44	1.33
24	c	512	CLA	O2D-CGD	3.80	1.42	1.33
24	b	604	CLA	CHC-C1C	3.80	1.46	1.35
24	b	613	CLA	C3D-C2D	3.81	1.48	1.39
24	b	604	CLA	OBD-CAD	3.81	1.27	1.22
24	B	607	CLA	C3C-C2C	3.82	1.44	1.36
24	B	609	CLA	C3B-C2B	3.83	1.45	1.40
24	c	512	CLA	CHC-C1C	3.83	1.46	1.35
24	C	507	CLA	C3C-C2C	3.83	1.44	1.36
24	c	513	CLA	O2D-CGD	3.84	1.42	1.33
24	b	614	CLA	CHB-C4A	3.85	1.38	1.33
29	j	101	LMG	O7-C10	3.87	1.45	1.34
24	A	607	CLA	CHC-C1C	3.87	1.46	1.35
28	x	101	SQD	O47-C7	3.88	1.45	1.34
24	b	604	CLA	C3B-C2B	3.88	1.45	1.40
24	b	616	CLA	CHB-C4A	3.88	1.38	1.33
24	c	504	CLA	C3C-C2C	3.89	1.45	1.36
24	B	604	CLA	OBD-CAD	3.90	1.28	1.22
24	d	405	CLA	C3C-C2C	3.90	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	C3C-C2C	3.90	1.45	1.36
24	B	616	CLA	OBD-CAD	3.90	1.28	1.22
25	D	401	PHO	CHB-C1B	3.90	1.46	1.38
24	a	407	CLA	C3C-C2C	3.90	1.45	1.36
25	D	401	PHO	CHD-C1D	3.91	1.46	1.38
24	B	602	CLA	C3D-C2D	3.91	1.48	1.39
25	A	608	PHO	CHC-C1C	3.91	1.46	1.38
24	C	511	CLA	C1B-CHB	3.92	1.50	1.40
40	h	104	DGD	O5D-C1E	3.92	1.47	1.40
24	C	502	CLA	CHC-C1C	3.93	1.46	1.35
24	d	403	CLA	C3B-C2B	3.93	1.45	1.40
24	B	604	CLA	C3D-C2D	3.95	1.48	1.39
24	D	403	CLA	C3C-C2C	3.96	1.45	1.36
24	D	405	CLA	CHC-C1C	3.96	1.46	1.35
24	b	610	CLA	CHC-C1C	3.96	1.46	1.35
24	b	609	CLA	C3C-C2C	3.96	1.45	1.36
24	B	612	CLA	CHC-C1C	3.97	1.46	1.35
24	B	614	CLA	C3C-C2C	3.97	1.45	1.36
24	C	507	CLA	C3B-C2B	3.97	1.45	1.40
24	c	513	CLA	C3C-C2C	3.98	1.45	1.36
24	B	617	CLA	OBD-CAD	3.98	1.28	1.22
24	B	614	CLA	CHC-C1C	3.99	1.46	1.35
24	c	508	CLA	C3B-C2B	3.99	1.45	1.40
28	l	102	SQD	O48-C23	3.99	1.45	1.33
24	b	617	CLA	OBD-CAD	3.99	1.28	1.22
25	d	401	PHO	CHB-C1B	4.00	1.46	1.38
28	A	616	SQD	O47-C7	4.00	1.45	1.34
24	B	603	CLA	C3C-C2C	4.00	1.45	1.36
24	C	510	CLA	C3C-C2C	4.00	1.45	1.36
24	C	508	CLA	CHC-C1C	4.01	1.47	1.35
25	a	409	PHO	CHD-C1D	4.01	1.46	1.38
24	b	608	CLA	C3D-C2D	4.02	1.48	1.39
24	B	606	CLA	O2D-CGD	4.03	1.43	1.33
24	b	611	CLA	C3B-C2B	4.03	1.45	1.40
24	d	405	CLA	C3D-C2D	4.03	1.48	1.39
32	E	101	LHG	O7-C7	4.04	1.46	1.34
24	c	503	CLA	CHC-C1C	4.04	1.47	1.35
29	z	101	LMG	O7-C10	4.04	1.46	1.34
24	C	502	CLA	C3C-C2C	4.04	1.45	1.36
24	D	405	CLA	C3D-C2D	4.05	1.48	1.39
24	B	607	CLA	CHC-C1C	4.05	1.47	1.35
24	C	512	CLA	O2A-CGA	4.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	C3B-C2B	4.06	1.45	1.40
24	C	503	CLA	C3B-C2B	4.06	1.45	1.40
28	A	616	SQD	O8-S	4.07	1.61	1.47
24	c	507	CLA	O2D-CGD	4.07	1.43	1.33
29	c	519	LMG	O8-C28	4.09	1.45	1.33
25	d	401	PHO	C3C-C2C	4.10	1.45	1.36
24	B	610	CLA	C3B-C2B	4.11	1.45	1.40
24	D	405	CLA	C3C-C2C	4.12	1.45	1.36
24	C	503	CLA	OBD-CAD	4.12	1.28	1.22
24	c	505	CLA	C3B-C2B	4.12	1.45	1.40
24	c	513	CLA	C3D-C2D	4.13	1.48	1.39
29	A	613	LMG	O7-C10	4.14	1.46	1.34
24	c	507	CLA	CHC-C1C	4.14	1.47	1.35
24	C	510	CLA	C3B-C2B	4.14	1.45	1.40
28	a	417	SQD	O47-C7	4.14	1.46	1.34
28	A	616	SQD	O48-C23	4.15	1.45	1.33
24	B	611	CLA	C3C-C2C	4.16	1.45	1.36
24	C	501	CLA	C3B-C2B	4.16	1.45	1.40
24	c	509	CLA	C3B-C2B	4.17	1.45	1.40
24	b	617	CLA	C3B-C2B	4.17	1.45	1.40
24	C	501	CLA	C3D-C2D	4.18	1.48	1.39
24	C	510	CLA	O2D-CGD	4.18	1.43	1.33
32	a	419	LHG	O7-C7	4.18	1.46	1.34
24	c	507	CLA	C3D-C2D	4.19	1.49	1.39
29	z	101	LMG	O8-C28	4.21	1.45	1.33
24	c	505	CLA	C3C-C2C	4.21	1.45	1.36
24	c	508	CLA	C3C-C2C	4.22	1.45	1.36
24	C	503	CLA	C3C-C2C	4.22	1.45	1.36
24	C	513	CLA	CHC-C1C	4.22	1.47	1.35
24	c	503	CLA	O2D-CGD	4.23	1.43	1.33
24	c	503	CLA	C3B-C2B	4.24	1.46	1.40
24	b	614	CLA	O2D-CGD	4.26	1.44	1.33
24	C	510	CLA	OBD-CAD	4.26	1.28	1.22
24	C	503	CLA	CHC-C1C	4.27	1.47	1.35
24	C	506	CLA	C3B-C2B	4.27	1.46	1.40
24	C	507	CLA	C3D-C2D	4.27	1.49	1.39
24	c	502	CLA	O2D-CGD	4.27	1.44	1.33
32	E	101	LHG	O8-C23	4.29	1.46	1.33
24	C	503	CLA	O2D-CGD	4.30	1.44	1.33
24	C	511	CLA	C3B-C2B	4.30	1.46	1.40
24	B	608	CLA	C3B-C2B	4.30	1.46	1.40
24	C	504	CLA	OBD-CAD	4.30	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	401	PHO	CHC-C1C	4.30	1.47	1.38
24	c	510	CLA	C3D-C2D	4.31	1.49	1.39
24	C	512	CLA	CHC-C1C	4.31	1.47	1.35
24	C	501	CLA	C3C-C2C	4.31	1.46	1.36
24	b	604	CLA	C3C-C2C	4.31	1.46	1.36
24	b	615	CLA	OBD-CAD	4.34	1.28	1.22
24	B	617	CLA	C3B-C2B	4.34	1.46	1.40
24	a	407	CLA	OBD-CAD	4.35	1.28	1.22
24	b	605	CLA	CHC-C1C	4.35	1.48	1.35
24	c	512	CLA	OBD-CAD	4.35	1.28	1.22
24	c	512	CLA	C3C-C2C	4.36	1.46	1.36
24	C	511	CLA	C3C-C2C	4.36	1.46	1.36
24	b	603	CLA	CHC-C1C	4.37	1.48	1.35
24	d	403	CLA	CHC-C1C	4.39	1.48	1.35
29	c	520	LMG	O7-C10	4.39	1.47	1.34
24	B	613	CLA	CHC-C1C	4.40	1.48	1.35
32	e	101	LHG	O7-C7	4.40	1.47	1.34
24	c	512	CLA	C3D-C2D	4.40	1.49	1.39
29	B	634	LMG	O7-C10	4.41	1.47	1.34
28	a	413	SQD	O8-S	4.42	1.62	1.47
24	C	512	CLA	C3D-C2D	4.42	1.49	1.39
24	a	408	CLA	OBD-CAD	4.43	1.28	1.22
24	c	504	CLA	C3D-C2D	4.44	1.49	1.39
24	B	603	CLA	CHC-C1C	4.45	1.48	1.35
28	A	612	SQD	O8-S	4.46	1.62	1.47
24	d	404	CLA	CHC-C1C	4.47	1.48	1.35
24	d	405	CLA	OBD-CAD	4.48	1.28	1.22
24	B	611	CLA	C3D-C2D	4.48	1.49	1.39
24	b	611	CLA	C3C-C2C	4.48	1.46	1.36
28	a	424	SQD	O48-C23	4.48	1.46	1.33
24	c	512	CLA	C3B-C2B	4.49	1.46	1.40
28	a	417	SQD	O8-S	4.50	1.62	1.47
24	c	507	CLA	C3C-C2C	4.50	1.46	1.36
24	C	507	CLA	O2D-CGD	4.50	1.44	1.33
24	B	612	CLA	CHB-C4A	4.52	1.39	1.33
24	C	505	CLA	C3C-C2C	4.53	1.46	1.36
24	c	511	CLA	OBD-CAD	4.54	1.28	1.22
29	d	412	LMG	O8-C28	4.55	1.46	1.33
28	a	424	SQD	O47-C7	4.55	1.47	1.34
24	b	608	CLA	C3C-C2C	4.58	1.46	1.36
24	B	613	CLA	OBD-CAD	4.59	1.29	1.22
32	e	101	LHG	O8-C23	4.60	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	618	LHG	O8-C23	4.61	1.46	1.33
40	D	408	DGD	O1G-C1A	4.61	1.46	1.33
24	D	404	CLA	CHB-C4A	4.63	1.39	1.33
28	F	104	SQD	O47-C7	4.65	1.47	1.34
28	F	104	SQD	O8-S	4.67	1.63	1.47
24	b	603	CLA	OBD-CAD	4.67	1.29	1.22
28	a	417	SQD	O48-C23	4.68	1.47	1.33
24	b	616	CLA	C3C-C2C	4.68	1.46	1.36
24	C	506	CLA	O2D-CGD	4.69	1.45	1.33
28	b	633	SQD	O48-C23	4.69	1.47	1.33
24	B	614	CLA	OBD-CAD	4.70	1.29	1.22
28	h	105	SQD	O47-C7	4.70	1.47	1.34
24	b	615	CLA	O2A-CGA	4.71	1.47	1.33
29	B	634	LMG	O8-C28	4.72	1.47	1.33
32	A	618	LHG	O7-C7	4.73	1.48	1.34
29	B	621	LMG	O8-C28	4.73	1.47	1.33
28	A	622	SQD	O48-C23	4.74	1.47	1.33
24	d	403	CLA	OBD-CAD	4.74	1.29	1.22
24	b	610	CLA	O2D-CGD	4.74	1.45	1.33
28	A	622	SQD	O47-C7	4.75	1.48	1.34
29	c	520	LMG	O8-C28	4.75	1.47	1.33
24	A	606	CLA	C3C-C2C	4.78	1.47	1.36
24	C	501	CLA	OBD-CAD	4.78	1.29	1.22
29	C	519	LMG	O8-C28	4.80	1.47	1.33
29	C	520	LMG	O7-C10	4.81	1.48	1.34
25	a	409	PHO	CHB-C1B	4.82	1.48	1.38
24	c	513	CLA	OBD-CAD	4.83	1.29	1.22
24	C	511	CLA	C3D-C2D	4.83	1.50	1.39
32	a	419	LHG	O8-C23	4.83	1.47	1.33
28	x	101	SQD	O8-S	4.85	1.63	1.47
28	h	105	SQD	O48-C23	4.86	1.47	1.33
28	b	633	SQD	O47-C7	4.88	1.48	1.34
24	C	509	CLA	OBD-CAD	4.88	1.29	1.22
24	b	616	CLA	C3D-C2D	4.89	1.50	1.39
24	b	612	CLA	C3B-C2B	4.89	1.46	1.40
24	a	410	CLA	CHC-C1C	4.91	1.49	1.35
28	a	424	SQD	O8-S	4.92	1.64	1.47
40	d	408	DGD	O1G-C1A	4.93	1.47	1.33
28	A	622	SQD	O8-S	4.98	1.64	1.47
24	B	615	CLA	CHC-C1C	5.01	1.50	1.35
24	b	605	CLA	C2-C3	5.05	1.45	1.33
29	C	520	LMG	O8-C28	5.05	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C3B-C2B	5.06	1.47	1.40
28	x	101	SQD	O48-C23	5.07	1.48	1.33
28	h	105	SQD	O8-S	5.11	1.64	1.47
28	b	633	SQD	O8-S	5.13	1.64	1.47
38	c	530	HTG	O2-C2	5.15	1.54	1.43
29	C	526	LMG	O7-C10	5.17	1.49	1.34
24	B	605	CLA	C2-C3	5.18	1.45	1.33
24	c	510	CLA	C3B-C2B	5.19	1.47	1.40
24	b	610	CLA	OBD-CAD	5.21	1.29	1.22
24	c	510	CLA	OBD-CAD	5.24	1.29	1.22
24	C	508	CLA	C3C-C2C	5.26	1.48	1.36
24	b	614	CLA	C3C-C2C	5.29	1.48	1.36
24	b	602	CLA	O2A-CGA	5.29	1.48	1.33
24	c	501	CLA	C3B-C2B	5.30	1.47	1.40
24	b	613	CLA	OBD-CAD	5.31	1.30	1.22
24	C	508	CLA	C3B-C2B	5.35	1.47	1.40
24	c	513	CLA	C3B-C2B	5.37	1.47	1.40
24	B	604	CLA	C3C-C2C	5.37	1.48	1.36
25	A	608	PHO	C3B-C2B	5.39	1.47	1.37
24	b	606	CLA	C3C-C2C	5.39	1.48	1.36
25	a	409	PHO	C3B-C2B	5.40	1.47	1.37
24	b	607	CLA	C3B-C2B	5.41	1.47	1.40
24	B	602	CLA	C3B-C2B	5.45	1.47	1.40
24	b	606	CLA	C2-C3	5.47	1.46	1.33
24	C	513	CLA	C3B-C2B	5.48	1.47	1.40
40	d	408	DGD	O2G-C1B	5.49	1.50	1.34
24	c	507	CLA	OBD-CAD	5.52	1.30	1.22
28	l	102	SQD	O8-S	5.52	1.66	1.47
24	c	509	CLA	OBD-CAD	5.55	1.30	1.22
24	b	606	CLA	O2D-CGD	5.56	1.47	1.33
24	b	602	CLA	O2D-CGD	5.57	1.47	1.33
28	F	104	SQD	O48-C23	5.57	1.49	1.33
24	A	606	CLA	OBD-CAD	5.74	1.30	1.22
24	B	603	CLA	OBD-CAD	5.79	1.30	1.22
24	b	616	CLA	OBD-CAD	5.79	1.30	1.22
27	A	611	PL9	C7-C3	5.87	1.57	1.51
24	B	602	CLA	O2A-CGA	5.87	1.50	1.33
40	D	408	DGD	O2G-C1B	5.90	1.51	1.34
24	B	606	CLA	C2-C3	5.93	1.47	1.33
24	C	505	CLA	OBD-CAD	6.60	1.31	1.22
25	D	401	PHO	C3B-C2B	6.79	1.50	1.37
24	b	614	CLA	OBD-CAD	6.81	1.32	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	412	PL9	C7-C3	7.44	1.59	1.51
24	D	403	CLA	OBD-CAD	7.82	1.33	1.22

All (2258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	C1C-NC-C4C	-13.51	99.29	107.06
24	b	605	CLA	C1C-NC-C4C	-13.35	99.38	107.06
24	B	610	CLA	C1C-NC-C4C	-13.26	99.43	107.06
24	b	617	CLA	C1C-NC-C4C	-12.77	99.71	107.06
24	B	612	CLA	C1C-NC-C4C	-12.75	99.72	107.06
24	b	610	CLA	C1C-NC-C4C	-12.40	99.93	107.06
24	C	507	CLA	C1C-NC-C4C	-11.98	100.17	107.06
24	B	605	CLA	C1C-NC-C4C	-11.87	100.23	107.06
24	c	508	CLA	C1C-NC-C4C	-11.76	100.29	107.06
24	b	607	CLA	C1C-NC-C4C	-11.67	100.34	107.06
24	b	613	CLA	C1C-NC-C4C	-11.60	100.38	107.06
24	d	404	CLA	C1C-NC-C4C	-11.59	100.39	107.06
24	B	616	CLA	C1C-NC-C4C	-11.51	100.43	107.06
24	B	602	CLA	C1C-NC-C4C	-11.38	100.51	107.06
24	B	609	CLA	C1C-NC-C4C	-11.33	100.54	107.06
24	C	506	CLA	C1C-NC-C4C	-11.32	100.54	107.06
24	D	404	CLA	C1C-NC-C4C	-11.28	100.57	107.06
24	A	607	CLA	C1C-NC-C4C	-11.27	100.57	107.06
24	c	505	CLA	C1C-NC-C4C	-11.25	100.58	107.06
24	A	609	CLA	C1C-NC-C4C	-11.20	100.61	107.06
24	b	609	CLA	C1C-NC-C4C	-11.11	100.66	107.06
24	a	408	CLA	C1C-NC-C4C	-11.10	100.67	107.06
24	C	505	CLA	C1C-NC-C4C	-10.97	100.75	107.06
24	B	607	CLA	C1C-NC-C4C	-10.92	100.77	107.06
24	b	611	CLA	C1C-NC-C4C	-10.75	100.87	107.06
24	C	501	CLA	C1C-NC-C4C	-10.71	100.89	107.06
24	C	513	CLA	C1C-NC-C4C	-10.65	100.93	107.06
24	c	513	CLA	C1C-NC-C4C	-10.54	100.99	107.06
24	a	410	CLA	C1C-NC-C4C	-10.51	101.01	107.06
24	C	509	CLA	C1C-NC-C4C	-10.48	101.03	107.06
24	B	608	CLA	C1C-NC-C4C	-10.46	101.04	107.06
24	B	614	CLA	C1C-NC-C4C	-10.40	101.08	107.06
24	b	612	CLA	C1C-NC-C4C	-10.34	101.11	107.06
24	c	511	CLA	C1C-NC-C4C	-10.20	101.19	107.06
24	c	509	CLA	C1C-NC-C4C	-10.17	101.20	107.06
24	C	503	CLA	C1C-NC-C4C	-10.16	101.21	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C1C-NC-C4C	-10.12	101.23	107.06
24	b	602	CLA	C1C-NC-C4C	-10.11	101.24	107.06
24	c	503	CLA	C1C-NC-C4C	-10.10	101.25	107.06
24	c	512	CLA	C1C-NC-C4C	-10.09	101.25	107.06
24	b	614	CLA	C1C-NC-C4C	-9.93	101.34	107.06
24	C	508	CLA	C1C-NC-C4C	-9.91	101.36	107.06
24	C	512	CLA	C1C-NC-C4C	-9.90	101.36	107.06
24	b	603	CLA	C1C-NC-C4C	-9.82	101.41	107.06
24	b	615	CLA	C1C-NC-C4C	-9.72	101.46	107.06
24	b	604	CLA	C1C-NC-C4C	-9.70	101.47	107.06
24	c	510	CLA	C1C-NC-C4C	-9.67	101.49	107.06
24	c	501	CLA	C1C-NC-C4C	-9.65	101.51	107.06
24	c	507	CLA	C1C-NC-C4C	-9.52	101.58	107.06
24	c	504	CLA	C1C-NC-C4C	-9.47	101.61	107.06
24	B	617	CLA	C1C-NC-C4C	-9.44	101.63	107.06
24	D	403	CLA	C1C-NC-C4C	-9.38	101.66	107.06
24	C	510	CLA	C1C-NC-C4C	-9.18	101.78	107.06
24	c	502	CLA	C1C-NC-C4C	-9.17	101.78	107.06
24	B	615	CLA	C1C-NC-C4C	-9.14	101.80	107.06
24	D	405	CLA	C1C-NC-C4C	-9.04	101.85	107.06
24	A	606	CLA	C1C-NC-C4C	-8.98	101.89	107.06
24	C	504	CLA	C1C-NC-C4C	-8.93	101.92	107.06
24	c	506	CLA	C1C-NC-C4C	-8.92	101.93	107.06
24	b	616	CLA	C1C-NC-C4C	-8.87	101.95	107.06
24	a	407	CLA	C1C-NC-C4C	-8.83	101.97	107.06
24	B	603	CLA	C1C-NC-C4C	-8.47	102.18	107.06
24	b	606	CLA	C1C-NC-C4C	-8.46	102.19	107.06
24	d	405	CLA	C1C-NC-C4C	-8.35	102.25	107.06
38	V	204	HTG	O5-C1-C2	-8.13	99.14	110.28
26	d	406	BCR	C40-C30-C25	-8.07	97.22	110.31
24	B	613	CLA	C1C-NC-C4C	-8.02	102.44	107.06
24	C	511	CLA	C1C-NC-C4C	-8.02	102.44	107.06
24	B	604	CLA	C1C-NC-C4C	-8.01	102.45	107.06
24	B	605	CLA	C5-C3-C2	-7.99	104.74	121.10
24	C	501	CLA	O2D-CGD-O1D	-7.68	108.37	123.82
24	b	608	CLA	C1C-NC-C4C	-7.58	102.69	107.06
24	d	403	CLA	C1C-NC-C4C	-7.53	102.72	107.06
26	D	406	BCR	C40-C30-C25	-7.31	98.45	110.31
28	A	612	SQD	C1-O5-C5	-7.15	100.24	113.72
24	B	605	CLA	C1-C2-C3	-7.15	112.78	125.96
28	A	612	SQD	C1-C2-C3	-6.88	97.20	109.98
24	C	502	CLA	C1C-NC-C4C	-6.85	103.11	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	E	113	HEM	C1D-C2D-C3D	-6.48	102.49	107.00
24	b	605	CLA	C5-C3-C2	-6.39	108.02	121.10
26	C	525	BCR	C7-C8-C9	-6.27	116.79	126.21
24	d	404	CLA	C1C-C2C-C3C	-6.26	99.97	106.92
24	c	513	CLA	CHD-C4C-C3C	-5.97	115.93	124.92
24	c	501	CLA	O2D-CGD-O1D	-5.93	111.89	123.82
32	D	409	LHG	O8-C23-O10	-5.83	109.06	123.55
24	b	605	CLA	C1-C2-C3	-5.82	115.23	125.96
24	b	606	CLA	C5-C3-C2	-5.75	109.34	121.10
24	C	503	CLA	CHD-C4C-C3C	-5.70	116.33	124.92
24	c	504	CLA	C1C-C2C-C3C	-5.65	100.65	106.92
24	b	616	CLA	C1C-C2C-C3C	-5.64	100.67	106.92
28	a	413	SQD	C1-O5-C5	-5.62	103.13	113.72
24	B	607	CLA	C1C-C2C-C3C	-5.61	100.69	106.92
26	k	101	BCR	C39-C30-C25	-5.57	101.28	110.31
25	A	608	PHO	C4C-C3C-C2C	-5.49	100.65	106.81
24	B	602	CLA	CHD-C4C-C3C	-5.44	116.72	124.92
24	b	613	CLA	CHD-C4C-C3C	-5.43	116.73	124.92
29	C	526	LMG	C1-C2-C3	-5.42	99.90	109.98
24	b	605	CLA	C4-C3-C5	-5.42	105.88	115.29
24	C	504	CLA	C1C-C2C-C3C	-5.41	100.92	106.92
38	V	204	HTG	C1-O5-C5	-5.37	102.35	112.69
28	b	633	SQD	O5-C1-C2	-5.33	100.02	110.30
24	D	403	CLA	C1C-C2C-C3C	-5.33	101.01	106.92
24	B	604	CLA	O2D-CGD-O1D	-5.31	113.13	123.82
29	B	621	LMG	O7-C10-O9	-5.27	110.53	123.68
24	B	615	CLA	CHD-C4C-C3C	-5.26	117.00	124.92
24	B	611	CLA	CHD-C4C-C3C	-5.23	117.03	124.92
24	B	612	CLA	C1C-C2C-C3C	-5.21	101.14	106.92
24	C	506	CLA	C1C-C2C-C3C	-5.20	101.15	106.92
24	C	501	CLA	C1C-C2C-C3C	-5.20	101.16	106.92
26	b	618	BCR	C7-C8-C9	-5.17	118.45	126.21
24	C	508	CLA	C1C-C2C-C3C	-5.16	101.19	106.92
24	b	603	CLA	CHD-C4C-C3C	-5.15	117.16	124.92
25	d	401	PHO	C4C-C3C-C2C	-5.14	101.04	106.81
24	b	602	CLA	CHD-C4C-C3C	-5.13	117.19	124.92
24	B	606	CLA	CHD-C4C-C3C	-5.12	117.20	124.92
28	x	101	SQD	C5-C6-S	-5.08	107.25	114.34
24	c	511	CLA	C1C-C2C-C3C	-5.08	101.28	106.92
29	b	621	LMG	O7-C10-O9	-4.95	111.33	123.68
28	a	413	SQD	C1-C2-C3	-4.93	100.81	109.98
24	b	612	CLA	CHD-C4C-C3C	-4.92	117.51	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	501	CLA	C1C-C2C-C3C	-4.90	101.48	106.92
24	b	612	CLA	C1C-C2C-C3C	-4.86	101.53	106.92
32	d	409	LHG	O8-C23-O10	-4.85	111.50	123.55
29	b	621	LMG	O8-C28-O10	-4.85	111.50	123.55
24	b	610	CLA	O2D-CGD-O1D	-4.84	114.08	123.82
24	B	603	CLA	CHD-C4C-C3C	-4.84	117.62	124.92
24	c	506	CLA	CHD-C4C-C3C	-4.82	117.65	124.92
28	A	612	SQD	O7-S-C6	-4.81	102.72	106.83
24	C	507	CLA	CHD-C4C-C3C	-4.80	117.69	124.92
24	B	606	CLA	C5-C3-C2	-4.79	111.30	121.10
24	c	513	CLA	C1C-C2C-C3C	-4.78	101.61	106.92
26	B	619	BCR	C40-C30-C25	-4.78	102.55	110.31
24	b	606	CLA	CHD-C4C-C3C	-4.76	117.75	124.92
25	D	401	PHO	C4C-C3C-C2C	-4.69	101.54	106.81
26	C	514	BCR	C23-C24-C25	-4.69	114.12	127.25
24	c	503	CLA	CHD-C4C-C3C	-4.69	117.85	124.92
24	B	609	CLA	CHD-C4C-C3C	-4.68	117.86	124.92
24	b	617	CLA	CHD-C4C-C3C	-4.68	117.87	124.92
24	c	502	CLA	C1C-C2C-C3C	-4.67	101.73	106.92
24	d	405	CLA	CHD-C4C-C3C	-4.66	117.89	124.92
27	A	611	PL9	C7-C8-C9	-4.64	118.95	126.71
24	c	505	CLA	CHD-C4C-C3C	-4.64	117.93	124.92
24	B	606	CLA	C4-C3-C2	-4.62	111.36	123.69
24	b	613	CLA	C4C-C3C-C2C	-4.59	99.86	106.91
24	B	611	CLA	C4C-C3C-C2C	-4.59	99.87	106.91
26	T	102	BCR	C20-C21-C22	-4.58	120.77	127.31
24	B	607	CLA	CHD-C4C-C3C	-4.58	118.01	124.92
24	B	602	CLA	OBD-CAD-C3D	-4.58	119.59	128.03
41	E	113	HEM	CBD-CAD-C3D	-4.58	103.74	112.47
26	C	514	BCR	C24-C23-C22	-4.57	119.35	126.21
24	c	508	CLA	C1C-C2C-C3C	-4.56	101.86	106.92
24	c	507	CLA	CHD-C4C-C3C	-4.54	118.07	124.92
24	c	512	CLA	C1C-C2C-C3C	-4.54	101.88	106.92
24	c	505	CLA	C4C-C3C-C2C	-4.52	99.97	106.91
24	c	511	CLA	CHD-C4C-C3C	-4.52	118.10	124.92
24	B	604	CLA	C1C-C2C-C3C	-4.52	101.91	106.92
24	b	605	CLA	C4-C3-C2	-4.50	111.69	123.69
24	b	603	CLA	O2D-CGD-O1D	-4.49	114.79	123.82
24	C	506	CLA	CHD-C4C-C3C	-4.49	118.15	124.92
26	C	514	BCR	C7-C8-C9	-4.49	119.47	126.21
24	c	502	CLA	CHD-C4C-C3C	-4.47	118.17	124.92
24	B	606	CLA	C1-C2-C3	-4.46	117.74	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	CHD-C4C-C3C	-4.45	118.21	124.92
24	C	511	CLA	CHD-C4C-C3C	-4.42	118.25	124.92
24	d	403	CLA	CHD-C4C-C3C	-4.42	118.26	124.92
24	B	604	CLA	CHD-C4C-C3C	-4.42	118.26	124.92
26	t	102	BCR	C39-C30-C25	-4.41	103.15	110.31
40	C	517	DGD	O2G-C1B-O1B	-4.41	112.68	123.68
24	B	612	CLA	CHD-C4C-C3C	-4.39	118.30	124.92
26	T	102	BCR	C7-C8-C9	-4.38	119.64	126.21
24	b	615	CLA	O2D-CGD-O1D	-4.37	115.03	123.82
28	a	413	SQD	O5-C1-C2	-4.37	101.87	110.30
41	e	107	HEM	CBA-CAA-C2A	-4.36	104.16	112.48
26	d	406	BCR	C30-C25-C26	-4.36	116.47	122.59
24	B	606	CLA	C4C-C3C-C2C	-4.35	100.24	106.91
24	a	408	CLA	CHD-C4C-C3C	-4.34	118.38	124.92
24	c	509	CLA	CHD-C4C-C3C	-4.34	118.38	124.92
28	a	417	SQD	C5-C6-S	-4.33	108.30	114.34
24	C	513	CLA	CHD-C4C-C3C	-4.33	118.39	124.92
24	B	610	CLA	C1C-C2C-C3C	-4.33	102.12	106.92
31	M	101	LMT	O2B-C2B-C1B	-4.32	100.99	110.03
26	C	515	BCR	C3-C4-C5	-4.32	106.36	113.78
24	b	616	CLA	C1B-CHB-C4A	-4.29	121.62	130.12
24	C	507	CLA	C1C-C2C-C3C	-4.28	102.17	106.92
26	h	103	BCR	C38-C26-C25	-4.26	119.74	124.51
24	B	615	CLA	O2A-CGA-O1A	-4.25	113.01	123.55
24	b	617	CLA	C4C-C3C-C2C	-4.25	100.40	106.91
26	c	514	BCR	C7-C8-C9	-4.24	119.84	126.21
26	c	515	BCR	C32-C1-C6	-4.23	103.44	110.31
24	D	404	CLA	C1C-C2C-C3C	-4.21	102.25	106.92
24	B	605	CLA	C6-C5-C3	-4.21	103.12	112.66
24	c	510	CLA	CHD-C4C-C3C	-4.21	118.58	124.92
24	A	607	CLA	CHD-C4C-C3C	-4.20	118.59	124.92
24	B	603	CLA	O2D-CGD-O1D	-4.19	115.39	123.82
24	b	617	CLA	O2A-CGA-O1A	-4.18	113.17	123.55
26	t	102	BCR	C38-C26-C25	-4.18	119.83	124.51
24	b	610	CLA	C4C-C3C-C2C	-4.17	100.51	106.91
24	b	602	CLA	C2A-C1A-CHA	-4.17	116.53	123.92
26	C	514	BCR	C28-C27-C26	-4.15	106.65	113.78
41	v	202	HEM	CBD-CAD-C3D	-4.14	104.57	112.47
24	c	512	CLA	CHD-C4C-C3C	-4.13	118.69	124.92
26	b	619	BCR	C28-C27-C26	-4.13	106.68	113.78
24	b	606	CLA	C4-C3-C2	-4.12	112.70	123.69
24	C	505	CLA	CHD-C4C-C3C	-4.12	118.71	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C1C-C2C-C3C	-4.11	102.36	106.92
24	B	608	CLA	C1C-C2C-C3C	-4.11	102.36	106.92
31	A	617	LMT	O5'-C1'-C2'	-4.10	102.38	110.30
24	C	509	CLA	C1C-C2C-C3C	-4.10	102.37	106.92
24	C	507	CLA	O1D-CGD-CBD	-4.10	117.24	124.60
24	b	605	CLA	C6-C5-C3	-4.09	103.38	112.66
24	B	616	CLA	CHD-C4C-C3C	-4.09	118.75	124.92
24	b	605	CLA	CHD-C4C-C3C	-4.09	118.75	124.92
24	C	502	CLA	C1C-C2C-C3C	-4.08	102.40	106.92
24	b	611	CLA	CHD-C4C-C3C	-4.06	118.79	124.92
24	b	609	CLA	CHD-C4C-C3C	-4.06	118.81	124.92
24	B	609	CLA	C1C-C2C-C3C	-4.05	102.43	106.92
31	m	102	LMT	C1'-O5'-C5'	-4.05	106.09	113.72
26	b	620	BCR	C40-C30-C25	-4.05	103.75	110.31
24	a	408	CLA	C4C-C3C-C2C	-4.04	100.71	106.91
24	C	505	CLA	O2D-CGD-O1D	-4.03	115.71	123.82
24	C	513	CLA	C2A-C1A-CHA	-4.02	116.80	123.92
26	c	527	BCR	C7-C8-C9	-4.01	120.18	126.21
31	m	102	LMT	O5'-C1'-O1'	-4.00	100.52	110.02
24	B	616	CLA	C1C-C2C-C3C	-4.00	102.49	106.92
24	B	603	CLA	C4C-C3C-C2C	-3.98	100.80	106.91
24	a	407	CLA	C1C-C2C-C3C	-3.98	102.51	106.92
26	C	514	BCR	C20-C21-C22	-3.98	121.63	127.31
24	B	617	CLA	CHD-C4C-C3C	-3.97	118.93	124.92
26	b	619	BCR	C40-C30-C25	-3.97	103.87	110.31
28	F	104	SQD	C5-C6-S	-3.97	108.81	114.34
24	b	605	CLA	C1C-C2C-C3C	-3.97	102.52	106.92
26	B	618	BCR	C7-C8-C9	-3.97	120.25	126.21
24	b	616	CLA	CHD-C4C-C3C	-3.96	118.94	124.92
28	b	633	SQD	O3-C3-C4	-3.96	101.75	110.36
24	b	602	CLA	C1C-C2C-C3C	-3.94	102.55	106.92
24	a	410	CLA	CHD-C4C-C3C	-3.94	118.98	124.92
24	D	405	CLA	CHD-C4C-C3C	-3.94	118.99	124.92
24	B	605	CLA	C4-C3-C2	-3.93	113.19	123.69
24	B	602	CLA	C1C-C2C-C3C	-3.93	102.56	106.92
26	d	406	BCR	C38-C26-C25	-3.93	120.11	124.51
27	a	412	PL9	O1-C4-C3	-3.92	116.26	120.71
24	c	512	CLA	C1-C2-C3	-3.92	118.73	125.96
24	C	501	CLA	CHD-C4C-C3C	-3.92	119.01	124.92
24	D	403	CLA	CHD-C4C-C3C	-3.92	119.02	124.92
26	D	406	BCR	C7-C8-C9	-3.91	120.33	126.21
24	b	610	CLA	CHD-C4C-C3C	-3.91	119.03	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C4C-C3C-C2C	-3.90	100.92	106.91
24	b	611	CLA	C1C-C2C-C3C	-3.90	102.59	106.92
24	D	404	CLA	C1B-CHB-C4A	-3.90	122.39	130.12
24	B	617	CLA	O2A-CGA-O1A	-3.90	113.86	123.55
24	b	615	CLA	CHD-C4C-C3C	-3.90	119.04	124.92
24	b	604	CLA	C1C-C2C-C3C	-3.89	102.60	106.92
26	b	620	BCR	C7-C8-C9	-3.89	120.37	126.21
41	E	113	HEM	CBA-CAA-C2A	-3.89	105.05	112.48
24	D	404	CLA	C3A-C2A-C1A	-3.89	95.52	101.34
26	d	406	BCR	C31-C1-C6	-3.88	104.01	110.31
24	b	614	CLA	CHD-C4C-C3C	-3.88	119.07	124.92
24	C	505	CLA	C4C-C3C-C2C	-3.88	100.96	106.91
24	C	513	CLA	C4C-C3C-C2C	-3.88	100.96	106.91
24	A	609	CLA	C1C-C2C-C3C	-3.87	102.62	106.92
24	b	607	CLA	C2A-C1A-CHA	-3.87	117.06	123.92
38	V	204	HTG	C1-C2-C3	-3.86	102.43	110.69
24	A	609	CLA	OBD-CAD-C3D	-3.85	120.93	128.03
24	B	608	CLA	CHD-C4C-C3C	-3.85	119.12	124.92
24	b	603	CLA	C4C-C3C-C2C	-3.85	101.01	106.91
41	V	203	HEM	CBD-CAD-C3D	-3.85	105.13	112.47
26	c	514	BCR	C24-C23-C22	-3.84	120.44	126.21
25	A	608	PHO	C1C-NC-C4C	-3.82	98.96	106.52
24	B	610	CLA	CHD-C4C-C3C	-3.81	119.17	124.92
24	b	609	CLA	C1C-C2C-C3C	-3.81	102.70	106.92
24	b	606	CLA	O2D-CGD-O1D	-3.80	116.17	123.82
26	b	618	BCR	C8-C7-C6	-3.80	116.61	127.25
24	c	504	CLA	C7-C6-C5	-3.79	102.57	113.11
25	d	401	PHO	C1C-NC-C4C	-3.79	99.02	106.52
24	D	404	CLA	C2A-C1A-CHA	-3.79	117.21	123.92
24	b	607	CLA	CHD-C4C-C3C	-3.78	119.23	124.92
24	C	509	CLA	CHD-C4C-C3C	-3.77	119.23	124.92
24	B	607	CLA	O2D-CGD-O1D	-3.77	116.24	123.82
27	A	611	PL9	C37-C36-C34	-3.77	100.19	112.93
31	b	622	LMT	O1B-C4'-C5'	-3.77	100.08	109.34
24	c	509	CLA	C4C-C3C-C2C	-3.77	101.13	106.91
32	d	410	LHG	O8-C23-O10	-3.76	114.22	123.55
24	B	612	CLA	C2A-C1A-CHA	-3.76	117.26	123.92
24	C	501	CLA	C2A-C1A-CHA	-3.75	117.26	123.92
24	C	502	CLA	OBD-CAD-C3D	-3.75	121.12	128.03
24	d	403	CLA	C4C-C3C-C2C	-3.75	101.16	106.91
26	a	411	BCR	C7-C8-C9	-3.74	120.60	126.21
24	c	501	CLA	CHD-C4C-C3C	-3.73	119.29	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	609	CLA	CHD-C4C-C3C	-3.73	119.30	124.92
24	B	606	CLA	C2A-C1A-CHA	-3.73	117.31	123.92
24	C	506	CLA	O2D-CGD-O1D	-3.72	116.33	123.82
26	C	525	BCR	C24-C23-C22	-3.72	120.62	126.21
31	B	622	LMT	O1B-C4'-C5'	-3.72	100.19	109.34
26	c	527	BCR	C24-C23-C22	-3.72	120.62	126.21
27	A	611	PL9	C7-C3-C4	-3.71	113.86	116.88
24	B	617	CLA	C1C-C2C-C3C	-3.71	102.81	106.92
24	b	606	CLA	C4C-C3C-C2C	-3.70	101.24	106.91
31	I	101	LMT	C2'-C3'-C4'	-3.69	101.94	109.61
40	C	518	DGD	O3G-C3G-C2G	-3.68	102.22	110.99
27	a	412	PL9	C2-C3-C4	-3.68	113.69	118.81
24	d	405	CLA	C4C-C3C-C2C	-3.68	101.27	106.91
24	b	615	CLA	O2A-CGA-O1A	-3.68	114.42	123.55
24	a	410	CLA	C1C-C2C-C3C	-3.67	102.84	106.92
25	d	401	PHO	O2D-CGD-O1D	-3.66	116.45	123.82
24	c	505	CLA	C2A-C1A-CHA	-3.66	117.44	123.92
26	c	515	BCR	C19-C18-C17	-3.64	113.36	118.94
26	c	515	BCR	C24-C23-C22	-3.63	120.76	126.21
26	c	515	BCR	C7-C8-C9	-3.63	120.76	126.21
24	C	507	CLA	C2A-C1A-CHA	-3.62	117.50	123.92
24	c	506	CLA	C4C-C3C-C2C	-3.62	101.36	106.91
24	C	502	CLA	CHD-C4C-C3C	-3.61	119.47	124.92
24	b	607	CLA	C1C-C2C-C3C	-3.61	102.91	106.92
27	A	611	PL9	O1-C4-C3	-3.61	116.61	120.71
26	h	103	BCR	C40-C30-C25	-3.61	104.45	110.31
24	b	602	CLA	OBD-CAD-C3D	-3.61	121.38	128.03
26	H	102	BCR	C7-C8-C9	-3.61	120.79	126.21
25	A	608	PHO	C3D-C2D-C1D	-3.60	100.49	105.82
24	c	501	CLA	C2A-C1A-CHA	-3.59	117.55	123.92
24	c	510	CLA	C4C-C3C-C2C	-3.59	101.40	106.91
24	D	405	CLA	C1C-C2C-C3C	-3.59	102.94	106.92
40	c	517	DGD	O2G-C1B-O1B	-3.58	114.73	123.68
24	C	513	CLA	OBD-CAD-C3D	-3.58	121.43	128.03
32	B	632	LHG	O7-C7-O9	-3.58	114.75	123.68
24	C	508	CLA	CHD-C4C-C3C	-3.57	119.54	124.92
24	C	512	CLA	CHD-C4C-C3C	-3.57	119.54	124.92
24	b	606	CLA	C1-C2-C3	-3.56	119.39	125.96
24	B	602	CLA	O2D-CGD-O1D	-3.56	116.66	123.82
24	b	604	CLA	CHD-C4C-C3C	-3.55	119.56	124.92
24	a	407	CLA	CHD-C4C-C3C	-3.55	119.56	124.92
24	B	615	CLA	O2D-CGD-O1D	-3.54	116.69	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	610	BCR	C7-C8-C9	-3.54	120.90	126.21
24	d	403	CLA	CBC-CAC-C3C	-3.52	102.41	112.41
26	H	102	BCR	C24-C23-C22	-3.51	120.94	126.21
26	c	514	BCR	C23-C24-C25	-3.51	117.43	127.25
26	d	406	BCR	C33-C5-C6	-3.51	120.58	124.51
38	h	101	HTG	O5-C1-S1	-3.50	100.89	110.15
41	v	202	HEM	CMA-C3A-C4A	-3.50	123.09	128.46
24	C	513	CLA	O2D-CGD-O1D	-3.50	116.79	123.82
24	B	604	CLA	C2A-C1A-CHA	-3.49	117.73	123.92
24	B	615	CLA	C1C-C2C-C3C	-3.49	103.05	106.92
24	c	513	CLA	C6-C5-C3	-3.49	104.75	112.66
25	D	401	PHO	C3B-C2B-C1B	-3.49	99.25	106.30
29	C	519	LMG	O7-C10-O9	-3.49	114.97	123.68
28	F	104	SQD	O5-C1-C2	-3.48	103.58	110.30
24	b	611	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
26	C	515	BCR	C7-C8-C9	-3.47	120.99	126.21
24	b	608	CLA	C4C-C3C-C2C	-3.47	101.58	106.91
25	a	409	PHO	C4C-C3C-C2C	-3.47	102.91	106.81
28	A	616	SQD	C1-O5-C5	-3.47	107.18	113.72
24	b	602	CLA	O2D-CGD-O1D	-3.47	116.85	123.82
24	b	614	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
24	b	611	CLA	O2A-CGA-O1A	-3.46	114.95	123.55
24	c	503	CLA	C2A-C1A-CHA	-3.46	117.79	123.92
26	C	525	BCR	C32-C1-C6	-3.46	104.70	110.31
29	d	412	LMG	O7-C10-O9	-3.45	115.08	123.68
40	C	516	DGD	O2G-C1B-O1B	-3.45	115.08	123.68
24	b	609	CLA	C4C-C3C-C2C	-3.45	101.62	106.91
29	J	101	LMG	O8-C28-O10	-3.44	115.01	123.55
24	b	604	CLA	O2D-CGD-O1D	-3.42	116.94	123.82
28	F	104	SQD	O8-S-O7	-3.42	103.53	111.37
24	D	405	CLA	C4C-C3C-C2C	-3.42	101.67	106.91
26	b	619	BCR	C38-C26-C25	-3.40	120.70	124.51
24	D	404	CLA	CHD-C4C-C3C	-3.40	119.80	124.92
24	B	613	CLA	CHD-C4C-C3C	-3.40	119.80	124.92
40	H	103	DGD	O3G-C1D-C2D	-3.39	102.70	108.23
38	b	631	HTG	O5-C1-C2	-3.39	105.64	110.28
24	c	507	CLA	C4C-C3C-C2C	-3.38	101.72	106.91
27	A	611	PL9	C2-C3-C4	-3.37	114.12	118.81
24	b	606	CLA	C6-C5-C3	-3.37	105.02	112.66
40	c	516	DGD	C3B-C2B-C1B	-3.36	101.31	113.58
24	B	611	CLA	OBD-CAD-C3D	-3.36	121.83	128.03
24	b	611	CLA	C4C-C3C-C2C	-3.36	101.75	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	OBD-CAD-C3D	-3.36	121.83	128.03
24	b	605	CLA	C4C-C3C-C2C	-3.34	101.78	106.91
24	c	512	CLA	CHC-C1C-C2C	-3.34	117.55	126.65
26	b	619	BCR	C37-C22-C21	-3.34	118.25	122.92
24	b	606	CLA	C1C-C2C-C3C	-3.33	103.22	106.92
24	D	405	CLA	C2A-C1A-CHA	-3.32	118.02	123.92
24	c	503	CLA	C1C-C2C-C3C	-3.32	103.23	106.92
26	B	618	BCR	C8-C7-C6	-3.32	117.95	127.25
38	a	418	HTG	O3-C3-C4	-3.32	103.13	110.36
26	t	102	BCR	C23-C22-C21	-3.32	113.85	118.94
24	d	405	CLA	C2A-C1A-CHA	-3.32	118.04	123.92
26	k	101	BCR	C38-C26-C25	-3.31	120.80	124.51
26	C	525	BCR	C20-C21-C22	-3.31	122.58	127.31
24	c	507	CLA	C2A-C1A-CHA	-3.31	118.06	123.92
29	a	414	LMG	C7-O1-C1	-3.31	106.98	113.76
31	b	622	LMT	O5'-C1'-O1'	-3.30	102.17	110.02
25	a	409	PHO	C1C-C2C-C3C	-3.30	102.68	106.51
38	c	522	HTG	O5-C1-C2	-3.30	105.75	110.28
24	C	507	CLA	O2A-CGA-O1A	-3.30	115.35	123.55
24	C	502	CLA	O2D-CGD-O1D	-3.30	117.18	123.82
24	B	614	CLA	C4C-C3C-C2C	-3.30	101.85	106.91
24	C	510	CLA	C4C-C3C-C2C	-3.29	101.87	106.91
26	T	102	BCR	C19-C18-C17	-3.28	113.90	118.94
24	c	507	CLA	C1C-C2C-C3C	-3.28	103.28	106.92
26	B	619	BCR	C29-C28-C27	-3.28	103.52	111.34
32	A	618	LHG	O8-C23-O10	-3.28	115.42	123.55
25	A	608	PHO	CHC-C1C-C2C	-3.27	118.11	125.62
24	b	607	CLA	CHC-C1C-C2C	-3.27	117.73	126.65
28	a	424	SQD	O48-C23-O10	-3.27	115.44	123.55
26	C	515	BCR	C15-C16-C17	-3.26	116.50	123.46
29	c	519	LMG	O1-C7-C8	-3.26	103.24	110.99
24	b	614	CLA	C1-C2-C3	-3.25	119.96	125.96
24	b	614	CLA	C4C-C3C-C2C	-3.25	101.93	106.91
28	F	104	SQD	O4-C4-C3	-3.25	103.29	110.36
28	a	417	SQD	C1-C2-C3	-3.25	103.94	109.98
40	h	104	DGD	C3E-C4E-C5E	-3.25	104.50	110.22
24	c	509	CLA	C16-C15-C13	-3.23	105.12	115.73
24	C	512	CLA	C4C-C3C-C2C	-3.23	101.96	106.91
24	D	403	CLA	CBC-CAC-C3C	-3.22	103.26	112.41
26	B	618	BCR	C16-C15-C14	-3.22	116.59	123.46
24	B	613	CLA	O2D-CGD-O1D	-3.21	117.36	123.82
24	d	405	CLA	C1C-C2C-C3C	-3.21	103.36	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	515	BCR	C24-C23-C22	-3.21	121.39	126.21
24	C	511	CLA	C1C-C2C-C3C	-3.21	103.36	106.92
28	A	612	SQD	O5-C1-C2	-3.21	104.10	110.30
41	V	203	HEM	C4A-C3A-C2A	-3.21	104.76	107.00
26	K	101	BCR	C37-C22-C21	-3.21	118.43	122.92
24	C	503	CLA	C2A-C1A-CHA	-3.21	118.23	123.92
24	B	611	CLA	O2D-CGD-O1D	-3.21	117.37	123.82
24	C	511	CLA	O2D-CGD-O1D	-3.20	117.38	123.82
31	M	101	LMT	C1'-O5'-C5'	-3.20	107.69	113.72
24	C	512	CLA	C2A-C1A-CHA	-3.19	118.26	123.92
26	K	101	BCR	C39-C30-C25	-3.19	105.14	110.31
24	b	606	CLA	C2A-C1A-CHA	-3.18	118.27	123.92
26	C	514	BCR	C8-C7-C6	-3.18	118.35	127.25
24	b	603	CLA	O2A-CGA-O1A	-3.17	115.67	123.55
24	B	614	CLA	CHD-C4C-C3C	-3.17	120.13	124.92
26	b	619	BCR	C29-C28-C27	-3.17	103.80	111.34
24	a	408	CLA	C1C-C2C-C3C	-3.17	103.41	106.92
29	c	519	LMG	O8-C28-O10	-3.16	115.69	123.55
26	c	515	BCR	C38-C26-C25	-3.16	120.97	124.51
29	C	519	LMG	O8-C28-O10	-3.16	115.71	123.55
24	a	410	CLA	C2A-C1A-CHA	-3.16	118.32	123.92
26	h	103	BCR	C30-C25-C26	-3.15	118.16	122.59
24	a	410	CLA	C5-C3-C2	-3.15	114.65	121.10
24	b	607	CLA	O2A-CGA-O1A	-3.15	115.73	123.55
24	C	508	CLA	C2A-C1A-CHA	-3.15	118.33	123.92
24	a	410	CLA	C4C-C3C-C2C	-3.14	102.09	106.91
24	C	509	CLA	OBD-CAD-C3D	-3.14	122.24	128.03
26	B	620	BCR	C38-C26-C25	-3.14	120.99	124.51
26	h	103	BCR	C7-C8-C9	-3.14	121.50	126.21
40	c	517	DGD	O1G-C1A-O1A	-3.14	115.76	123.55
26	a	411	BCR	C37-C22-C21	-3.13	118.53	122.92
27	a	412	PL9	C37-C38-C39	-3.13	119.81	127.68
24	B	608	CLA	O1D-CGD-CBD	-3.13	118.97	124.60
26	b	619	BCR	C30-C25-C26	-3.13	118.19	122.59
40	h	104	DGD	O5D-C6D-C5D	-3.12	103.72	108.94
40	H	103	DGD	O1G-C1A-O1A	-3.12	115.81	123.55
40	h	104	DGD	O1G-C1A-O1A	-3.11	115.83	123.55
24	b	612	CLA	C2A-C1A-CHA	-3.11	118.41	123.92
24	b	616	CLA	C2A-C1A-CHA	-3.10	118.42	123.92
24	b	613	CLA	C2A-C1A-CHA	-3.10	118.42	123.92
40	D	408	DGD	O2G-C1B-O1B	-3.09	115.96	123.68
26	H	102	BCR	C40-C30-C25	-3.09	105.29	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	CHD-C4C-C3C	-3.09	120.26	124.92
38	h	101	HTG	C2'-C1'-S1	-3.09	102.37	112.45
26	A	610	BCR	C20-C21-C22	-3.08	122.91	127.31
24	B	614	CLA	O2A-CGA-O1A	-3.08	115.90	123.55
24	B	616	CLA	C11-C10-C8	-3.08	105.62	115.73
26	t	102	BCR	C7-C8-C9	-3.08	121.58	126.21
31	u	203	LMT	O1B-C1B-O5B	-3.08	103.22	110.70
24	C	508	CLA	O2D-CGD-O1D	-3.08	117.62	123.82
29	b	621	LMG	C1-O6-C5	-3.08	107.92	113.72
26	t	102	BCR	C12-C13-C14	-3.08	114.22	118.94
24	c	501	CLA	CBC-CAC-C3C	-3.07	103.69	112.41
24	c	508	CLA	O2D-CGD-O1D	-3.07	117.64	123.82
26	t	102	BCR	C15-C16-C17	-3.07	116.91	123.46
31	J	103	LMT	C1-O1'-C1'	-3.07	108.60	113.87
24	B	617	CLA	C4C-C3C-C2C	-3.07	102.21	106.91
28	a	417	SQD	O48-C23-O10	-3.06	115.95	123.55
24	A	609	CLA	O2A-CGA-O1A	-3.06	115.95	123.55
26	H	102	BCR	C37-C22-C21	-3.06	118.64	122.92
26	C	525	BCR	C38-C26-C25	-3.05	121.09	124.51
24	c	513	CLA	C2A-C1A-CHA	-3.05	118.51	123.92
25	a	409	PHO	C3D-C2D-C1D	-3.05	101.30	105.82
40	d	408	DGD	O2G-C1B-O1B	-3.05	116.07	123.68
24	b	612	CLA	CBC-CAC-C3C	-3.05	103.76	112.41
24	d	404	CLA	O2D-CGD-O1D	-3.04	117.69	123.82
26	H	102	BCR	C20-C21-C22	-3.04	122.97	127.31
24	a	410	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
24	c	512	CLA	O1D-CGD-CBD	-3.04	119.14	124.60
24	A	606	CLA	C1C-C2C-C3C	-3.04	103.55	106.92
24	A	606	CLA	C4C-C3C-C2C	-3.04	102.25	106.91
24	c	504	CLA	CHD-C4C-C3C	-3.03	120.34	124.92
32	D	409	LHG	O7-C7-O9	-3.03	116.11	123.68
38	c	523	HTG	O5-C1-C2	-3.03	106.12	110.28
26	c	514	BCR	C20-C21-C22	-3.03	122.99	127.31
24	d	404	CLA	CHD-C4C-C3C	-3.02	120.36	124.92
26	C	514	BCR	C30-C25-C26	-3.02	118.34	122.59
28	l	102	SQD	C1-C2-C3	-3.02	104.36	109.98
26	d	406	BCR	C28-C27-C26	-3.02	108.59	113.78
24	B	604	CLA	C4C-C3C-C2C	-3.01	102.28	106.91
24	B	615	CLA	C2A-C1A-CHA	-3.01	118.57	123.92
26	k	101	BCR	C23-C24-C25	-3.01	118.82	127.25
29	C	519	LMG	O10-C28-C29	-3.01	111.77	123.68
29	z	101	LMG	C1-C2-C3	-3.01	104.38	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	408	CLA	C2A-C1A-CHA	-3.01	118.59	123.92
31	M	101	LMT	O5'-C1'-O1'	-3.01	102.89	110.02
24	C	506	CLA	C2A-C1A-CHA	-3.01	118.59	123.92
28	F	104	SQD	C1-C2-C3	-3.00	104.39	109.98
24	B	616	CLA	C2A-C1A-CHA	-3.00	118.59	123.92
40	C	516	DGD	C3G-C2G-C1G	-3.00	105.08	111.86
24	c	511	CLA	C2A-C1A-CHA	-3.00	118.60	123.92
24	c	509	CLA	C2A-C1A-CHA	-3.00	118.61	123.92
24	c	501	CLA	OBD-CAD-C3D	-2.99	122.51	128.03
40	H	103	DGD	O5D-C6D-C5D	-2.99	103.94	108.94
24	B	605	CLA	C7-C6-C5	-2.99	104.80	113.11
24	A	607	CLA	C4C-C3C-C2C	-2.99	102.33	106.91
24	c	504	CLA	C2A-C1A-CHA	-2.98	118.63	123.92
24	b	606	CLA	OBD-CAD-C3D	-2.98	122.53	128.03
24	C	503	CLA	C1C-C2C-C3C	-2.98	103.62	106.92
28	A	622	SQD	O48-C23-O10	-2.98	116.16	123.55
24	b	609	CLA	C2A-C1A-CHA	-2.98	118.64	123.92
26	d	406	BCR	C1-C6-C5	-2.98	118.41	122.59
38	b	631	HTG	O3-C3-C2	-2.97	103.89	110.36
24	c	506	CLA	O2D-CGD-O1D	-2.97	117.84	123.82
26	T	102	BCR	C16-C17-C18	-2.97	123.07	127.31
24	b	617	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
26	H	102	BCR	C29-C28-C27	-2.97	104.28	111.34
24	C	512	CLA	OBD-CAD-C3D	-2.96	122.57	128.03
29	a	414	LMG	C8-O7-C10	-2.96	110.88	117.88
24	C	510	CLA	C1C-C2C-C3C	-2.96	103.64	106.92
26	C	514	BCR	C11-C10-C9	-2.96	123.09	127.31
24	b	610	CLA	C2A-C1A-CHA	-2.96	118.68	123.92
28	A	612	SQD	O47-C7-O49	-2.96	116.30	123.68
26	B	618	BCR	C33-C5-C6	-2.96	121.20	124.51
24	a	407	CLA	CHC-C1C-C2C	-2.95	118.60	126.65
26	b	620	BCR	C23-C24-C25	-2.95	118.99	127.25
24	A	607	CLA	C1C-C2C-C3C	-2.95	103.65	106.92
24	B	610	CLA	O2D-CGD-O1D	-2.95	117.89	123.82
24	b	603	CLA	C2A-C1A-CHA	-2.94	118.70	123.92
24	B	609	CLA	C4C-C3C-C2C	-2.94	102.40	106.91
24	B	616	CLA	C4C-C3C-C2C	-2.94	102.40	106.91
24	b	604	CLA	C2A-C1A-CHA	-2.93	118.72	123.92
26	c	514	BCR	C39-C30-C25	-2.93	105.56	110.31
26	C	514	BCR	C31-C1-C6	-2.93	105.56	110.31
26	h	103	BCR	C31-C1-C6	-2.93	105.56	110.31
24	c	503	CLA	O2A-CGA-O1A	-2.92	116.30	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	521	LMT	C2'-C3'-C4'	-2.92	103.55	109.61
31	M	101	LMT	C3'-C4'-C5'	-2.92	104.68	110.88
26	a	411	BCR	C28-C27-C26	-2.91	108.77	113.78
24	B	611	CLA	C14-C13-C15	-2.91	100.74	111.36
28	A	616	SQD	O48-C23-O10	-2.91	116.33	123.55
32	d	409	LHG	O7-C7-O9	-2.90	116.43	123.68
31	I	101	LMT	O3B-C3B-C2B	-2.90	104.04	110.36
24	C	505	CLA	C1C-C2C-C3C	-2.89	103.71	106.92
28	b	633	SQD	O48-C23-O10	-2.89	116.37	123.55
24	c	509	CLA	C1C-C2C-C3C	-2.89	103.71	106.92
24	b	611	CLA	O2D-CGD-O1D	-2.89	118.01	123.82
32	l	101	LHG	O8-C23-O10	-2.88	116.39	123.55
32	D	410	LHG	O8-C23-O10	-2.88	116.39	123.55
24	C	509	CLA	O2D-CGD-O1D	-2.88	118.02	123.82
24	D	404	CLA	O2D-CGD-O1D	-2.88	118.02	123.82
24	d	405	CLA	O2D-CGD-O1D	-2.88	118.02	123.82
24	B	617	CLA	C2A-C1A-CHA	-2.88	118.81	123.92
24	b	617	CLA	O2D-CGD-O1D	-2.88	118.03	123.82
26	C	515	BCR	C39-C30-C25	-2.87	105.65	110.31
26	A	610	BCR	C24-C23-C22	-2.87	121.89	126.21
26	D	406	BCR	C30-C25-C26	-2.87	118.55	122.59
24	B	611	CLA	O2A-CGA-O1A	-2.87	116.43	123.55
24	C	512	CLA	CHC-C1C-C2C	-2.86	118.85	126.65
31	M	101	LMT	O1'-C1-C2	-2.86	99.48	109.68
24	A	609	CLA	C2A-C1A-CHA	-2.86	118.85	123.92
26	c	515	BCR	C8-C7-C6	-2.85	119.26	127.25
24	c	510	CLA	C2A-C1A-CHA	-2.85	118.86	123.92
24	b	603	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
24	b	617	CLA	C2A-C1A-CHA	-2.85	118.86	123.92
25	D	401	PHO	C3D-C2D-C1D	-2.85	101.59	105.82
26	h	103	BCR	C29-C28-C27	-2.85	104.56	111.34
29	C	519	LMG	O1-C7-C8	-2.85	104.21	110.99
24	B	610	CLA	C2A-C1A-CHA	-2.85	118.87	123.92
24	D	403	CLA	CHC-C1C-C2C	-2.84	118.89	126.65
41	V	203	HEM	CMD-C2D-C1D	-2.84	124.10	128.46
24	B	614	CLA	C2A-C1A-CHA	-2.84	118.89	123.92
24	c	507	CLA	O2A-CGA-O1A	-2.83	116.51	123.55
24	C	501	CLA	CBC-CAC-C3C	-2.83	104.37	112.41
26	c	515	BCR	C1-C6-C5	-2.83	118.61	122.59
26	h	103	BCR	C37-C22-C21	-2.83	118.96	122.92
26	H	102	BCR	C31-C1-C6	-2.83	105.72	110.31
24	b	612	CLA	OBD-CAD-C3D	-2.83	122.82	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	CBC-CAC-C3C	-2.82	104.39	112.41
25	a	409	PHO	C1C-NC-C4C	-2.82	100.93	106.52
24	C	507	CLA	OBD-CAD-C3D	-2.81	122.84	128.03
31	B	622	LMT	C1-O1'-C1'	-2.81	109.04	113.87
24	B	608	CLA	C2A-C1A-CHA	-2.81	118.94	123.92
26	t	102	BCR	C24-C23-C22	-2.81	121.99	126.21
26	b	618	BCR	C16-C17-C18	-2.81	123.31	127.31
26	h	103	BCR	C24-C23-C22	-2.80	122.00	126.21
26	K	101	BCR	C38-C26-C25	-2.80	121.38	124.51
29	C	520	LMG	O3-C3-C4	-2.80	104.27	110.36
30	C	523	GOL	C3-C2-C1	-2.79	100.41	111.52
24	B	612	CLA	CHC-C1C-C2C	-2.79	119.03	126.65
26	k	101	BCR	C20-C21-C22	-2.79	123.33	127.31
24	c	506	CLA	C2A-C1A-CHA	-2.79	118.98	123.92
24	B	607	CLA	C2A-C1A-CHA	-2.79	118.98	123.92
24	A	607	CLA	CHC-C1C-C2C	-2.79	119.05	126.65
24	B	602	CLA	C2A-C1A-CHA	-2.79	118.98	123.92
40	H	103	DGD	C3E-C4E-C5E	-2.78	105.31	110.22
26	B	619	BCR	C30-C25-C26	-2.77	118.69	122.59
24	A	606	CLA	C2A-C1A-CHA	-2.77	119.00	123.92
24	b	612	CLA	C1-C2-C3	-2.77	120.86	125.96
24	B	605	CLA	CHD-C4C-C3C	-2.77	120.75	124.92
26	C	514	BCR	C39-C30-C25	-2.76	105.83	110.31
24	B	605	CLA	C4-C3-C5	-2.76	110.49	115.29
24	B	602	CLA	CHC-C1C-C2C	-2.76	119.12	126.65
24	C	507	CLA	C4C-C3C-C2C	-2.76	102.67	106.91
24	a	410	CLA	OBD-CAD-C3D	-2.75	122.95	128.03
26	a	411	BCR	C23-C24-C25	-2.75	119.54	127.25
24	B	606	CLA	C4-C3-C5	-2.75	110.52	115.29
24	c	505	CLA	O2D-CGD-O1D	-2.75	118.30	123.82
24	C	504	CLA	CHC-C1C-C2C	-2.74	119.17	126.65
31	J	103	LMT	O2'-C2'-C3'	-2.74	104.39	110.36
27	A	611	PL9	C37-C38-C39	-2.74	120.80	127.68
26	D	406	BCR	C37-C22-C21	-2.74	119.09	122.92
24	c	502	CLA	CHC-C1C-C2C	-2.74	119.18	126.65
26	T	102	BCR	C39-C30-C25	-2.74	105.87	110.31
24	c	503	CLA	OBD-CAD-C3D	-2.74	122.98	128.03
24	c	507	CLA	O1D-CGD-CBD	-2.74	119.69	124.60
24	c	504	CLA	CBC-CAC-C3C	-2.73	104.65	112.41
40	C	516	DGD	C4E-C3E-C2E	-2.73	106.02	110.84
28	A	612	SQD	O9-S-O7	-2.73	104.41	113.86
27	a	412	PL9	C16-C14-C13	-2.72	115.53	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	C4C-C3C-C2C	-2.71	102.74	106.91
24	b	611	CLA	C2A-C1A-CHA	-2.71	119.11	123.92
24	C	509	CLA	C2A-C1A-CHA	-2.71	119.12	123.92
24	b	611	CLA	OBD-CAD-C3D	-2.71	123.04	128.03
40	H	103	DGD	O5E-C6E-C5E	-2.71	102.23	111.34
26	A	610	BCR	C8-C7-C6	-2.71	119.68	127.25
24	b	608	CLA	CHD-C4C-C3C	-2.70	120.84	124.92
26	B	618	BCR	C24-C23-C22	-2.70	122.15	126.21
24	C	509	CLA	O2A-CGA-O1A	-2.70	116.84	123.55
24	B	605	CLA	O1D-CGD-CBD	-2.70	119.75	124.60
24	b	615	CLA	C2A-C1A-CHA	-2.69	119.14	123.92
26	b	618	BCR	C15-C16-C17	-2.69	117.71	123.46
31	M	101	LMT	C3B-C4B-C5B	-2.69	105.47	110.22
24	C	513	CLA	C5-C3-C2	-2.69	115.60	121.10
24	c	504	CLA	CHC-C1C-C2C	-2.69	119.32	126.65
26	H	102	BCR	C38-C26-C25	-2.69	121.50	124.51
24	C	509	CLA	CHC-C1C-C2C	-2.69	119.32	126.65
40	d	408	DGD	C3G-C2G-C1G	-2.69	105.80	111.86
26	t	102	BCR	C11-C10-C9	-2.69	123.48	127.31
24	d	403	CLA	CHC-C1C-C2C	-2.69	119.33	126.65
24	b	615	CLA	C1C-C2C-C3C	-2.68	103.94	106.92
24	B	611	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
25	A	608	PHO	CHD-C4C-C3C	-2.68	119.20	124.59
24	b	608	CLA	C2A-C1A-CHA	-2.68	119.17	123.92
40	d	408	DGD	O6D-C1D-C2D	-2.67	105.14	110.30
24	B	606	CLA	C6-C5-C3	-2.67	106.61	112.66
40	C	516	DGD	C3D-C4D-C5D	-2.67	105.51	110.22
24	d	405	CLA	C5-C3-C2	-2.66	115.65	121.10
26	A	610	BCR	C39-C30-C25	-2.66	105.99	110.31
25	d	401	PHO	O2A-CGA-O1A	-2.66	116.94	123.55
24	a	410	CLA	C1-C2-C3	-2.66	121.06	125.96
29	A	613	LMG	C7-O1-C1	-2.66	108.30	113.76
38	C	529	HTG	O5-C1-C2	-2.66	106.63	110.28
29	c	519	LMG	O7-C10-O9	-2.66	117.05	123.68
24	D	405	CLA	CHC-C1C-C2C	-2.65	119.41	126.65
24	c	511	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
26	A	610	BCR	C11-C10-C9	-2.64	123.54	127.31
24	C	510	CLA	O2A-CGA-O1A	-2.64	116.99	123.55
26	H	102	BCR	C16-C17-C18	-2.64	123.54	127.31
30	B	625	GOL	O2-C2-C3	-2.64	96.36	108.84
24	b	606	CLA	C4-C3-C5	-2.64	110.70	115.29
24	c	501	CLA	CHC-C1C-C2C	-2.64	119.45	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
24	B	610	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
24	c	510	CLA	C1C-C2C-C3C	-2.63	104.00	106.92
31	B	622	LMT	C6B-C5B-C4B	-2.63	106.84	113.00
24	D	405	CLA	OBD-CAD-C3D	-2.63	123.18	128.03
24	C	501	CLA	OBD-CAD-C3D	-2.63	123.18	128.03
26	c	514	BCR	C31-C1-C6	-2.63	106.05	110.31
26	h	103	BCR	C11-C10-C9	-2.63	123.56	127.31
24	c	513	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
31	t	103	LMT	O5'-C1'-O1'	-2.62	103.80	110.02
25	d	401	PHO	CHC-C1C-C2C	-2.62	119.61	125.62
24	b	604	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
26	h	103	BCR	C33-C5-C4	-2.62	108.49	113.45
24	b	616	CLA	C6-C5-C3	-2.61	106.74	112.66
24	a	408	CLA	C3A-C2A-C1A	-2.61	97.43	101.34
40	c	516	DGD	C1D-O6D-C5D	-2.61	108.80	113.72
28	a	413	SQD	O47-C7-O49	-2.61	117.17	123.68
24	D	404	CLA	CHC-C1C-C2C	-2.61	119.54	126.65
24	b	602	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
24	C	504	CLA	C7-C6-C5	-2.59	105.90	113.11
40	C	516	DGD	C1D-O6D-C5D	-2.59	108.83	113.72
26	t	102	BCR	C28-C27-C26	-2.59	109.32	113.78
24	a	408	CLA	CHC-C1C-C2C	-2.59	119.58	126.65
27	d	407	PL9	C11-C9-C8	-2.59	115.81	121.10
24	C	502	CLA	C2A-C1A-CHA	-2.58	119.34	123.92
24	B	605	CLA	OBD-CAD-C3D	-2.58	123.27	128.03
24	b	612	CLA	O2D-CGD-O1D	-2.58	118.63	123.82
31	M	101	LMT	O5B-C1B-C2B	-2.58	105.32	110.30
29	B	621	LMG	O8-C28-O10	-2.58	117.15	123.55
25	D	401	PHO	C1C-NC-C4C	-2.58	101.42	106.52
24	C	511	CLA	C4C-C3C-C2C	-2.58	102.96	106.91
24	B	608	CLA	C4C-C3C-C2C	-2.57	102.96	106.91
24	B	603	CLA	C16-C15-C13	-2.57	107.28	115.73
40	C	518	DGD	C6B-C5B-C4B	-2.57	101.20	114.45
24	c	512	CLA	C4C-C3C-C2C	-2.57	102.96	106.91
24	B	615	CLA	C4C-C3C-C2C	-2.57	102.96	106.91
32	d	411	LHG	O8-C23-O10	-2.57	117.18	123.55
24	b	611	CLA	C14-C13-C15	-2.57	102.00	111.36
25	d	401	PHO	C1C-C2C-C3C	-2.56	103.54	106.51
26	B	618	BCR	C20-C21-C22	-2.56	123.66	127.31
24	c	505	CLA	C1C-C2C-C3C	-2.55	104.09	106.92
29	B	634	LMG	O8-C28-O10	-2.55	117.22	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	102	BCR	C19-C18-C17	-2.55	115.03	118.94
27	d	407	PL9	C50-C49-C48	-2.55	114.97	122.65
28	a	413	SQD	C45-O47-C7	-2.54	111.86	117.88
24	a	407	CLA	C4C-C3C-C2C	-2.54	103.01	106.91
24	B	614	CLA	C1-C2-C3	-2.54	121.27	125.96
32	D	409	LHG	C11-C10-C9	-2.54	101.36	114.45
27	D	407	PL9	C40-C39-C38	-2.54	116.91	123.69
26	c	527	BCR	C37-C22-C21	-2.54	119.36	122.92
26	t	102	BCR	C7-C6-C5	-2.54	115.48	121.54
24	c	508	CLA	OBD-CAD-C3D	-2.54	123.35	128.03
24	B	612	CLA	C4C-C3C-C2C	-2.54	103.01	106.91
24	B	611	CLA	C2A-C1A-CHA	-2.54	119.42	123.92
24	c	502	CLA	OBD-CAD-C3D	-2.53	123.36	128.03
24	b	614	CLA	C7-C6-C5	-2.53	106.08	113.11
24	b	617	CLA	C1C-C2C-C3C	-2.53	104.11	106.92
26	c	527	BCR	C20-C21-C22	-2.52	123.71	127.31
24	c	512	CLA	C2A-C1A-CHA	-2.52	119.44	123.92
24	b	603	CLA	C1-C2-C3	-2.52	121.31	125.96
26	H	102	BCR	C16-C15-C14	-2.52	118.08	123.46
24	c	506	CLA	C1C-C2C-C3C	-2.52	104.12	106.92
24	d	405	CLA	C6-C7-C8	-2.52	107.46	115.73
25	d	401	PHO	CHD-C4C-C3C	-2.52	119.52	124.59
24	B	611	CLA	C20-C18-C19	-2.52	98.59	110.50
26	b	618	BCR	C20-C21-C22	-2.52	123.72	127.31
24	B	616	CLA	CHC-C1C-C2C	-2.51	119.80	126.65
24	b	606	CLA	O2A-CGA-O1A	-2.51	117.31	123.55
26	B	620	BCR	C23-C22-C21	-2.51	115.09	118.94
24	d	403	CLA	C2A-C1A-CHA	-2.50	119.48	123.92
38	a	418	HTG	C1-C2-C3	-2.50	105.34	110.69
27	a	412	PL9	O2-C1-C2	-2.50	115.93	121.77
24	B	613	CLA	C2A-C1A-CHA	-2.49	119.50	123.92
24	B	607	CLA	OBD-CAD-C3D	-2.49	123.43	128.03
24	d	405	CLA	OBD-CAD-C3D	-2.49	123.43	128.03
24	B	608	CLA	C1-C2-C3	-2.49	121.37	125.96
28	b	633	SQD	C1-C2-C3	-2.49	105.35	109.98
40	c	518	DGD	C3A-C2A-C1A	-2.49	104.50	113.58
26	c	527	BCR	C8-C7-C6	-2.49	120.29	127.25
28	l	102	SQD	C26-C25-C24	-2.49	104.13	113.24
24	b	613	CLA	OBD-CAD-C3D	-2.49	123.45	128.03
29	j	101	LMG	O8-C28-O10	-2.48	117.38	123.55
26	b	619	BCR	C8-C9-C10	-2.48	115.13	118.94
24	C	511	CLA	C2A-C1A-CHA	-2.48	119.52	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C8-C9-C10	-2.48	115.14	118.94
38	c	522	HTG	O2-C2-C1	-2.48	105.33	110.27
26	T	102	BCR	C11-C12-C13	-2.48	119.46	126.42
24	B	614	CLA	C1C-C2C-C3C	-2.48	104.18	106.92
24	B	602	CLA	O1A-CGA-CBA	-2.47	113.90	123.68
29	j	101	LMG	O2-C2-C1	-2.47	104.85	110.03
28	A	612	SQD	O4-C4-C3	-2.47	104.98	110.36
24	B	617	CLA	O1D-CGD-CBD	-2.47	120.16	124.60
25	A	608	PHO	CHD-C1D-ND	-2.47	119.80	124.64
38	B	624	HTG	O5-C5-C4	-2.47	105.11	109.66
24	C	501	CLA	CHC-C1C-C2C	-2.47	119.92	126.65
24	C	509	CLA	C4C-C3C-C2C	-2.47	103.12	106.91
31	m	102	LMT	O1'-C1-C2	-2.47	100.88	109.68
26	b	619	BCR	C16-C15-C14	-2.47	118.20	123.46
24	C	506	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
31	A	617	LMT	O1B-C1B-O5B	-2.46	104.71	110.70
26	B	619	BCR	C38-C26-C25	-2.46	121.75	124.51
28	b	633	SQD	C1-O5-C5	-2.46	109.08	113.72
29	B	621	LMG	C38-C37-C36	-2.46	101.78	114.45
25	a	409	PHO	CHC-C1C-C2C	-2.46	119.98	125.62
24	b	610	CLA	C1C-C2C-C3C	-2.46	104.19	106.92
26	H	102	BCR	C30-C25-C26	-2.45	119.14	122.59
26	C	525	BCR	C16-C17-C18	-2.45	123.81	127.31
26	c	514	BCR	C33-C5-C6	-2.45	121.77	124.51
24	a	407	CLA	O2A-CGA-O1A	-2.45	117.47	123.55
24	C	510	CLA	OBD-CAD-C3D	-2.45	123.52	128.03
24	b	611	CLA	CAA-CBA-CGA	-2.44	105.98	113.35
24	B	602	CLA	C4C-C3C-C2C	-2.44	103.16	106.91
24	C	510	CLA	C2A-C1A-CHA	-2.44	119.59	123.92
24	d	404	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
40	h	104	DGD	O4D-C4D-C3D	-2.44	105.05	110.36
24	b	608	CLA	CHC-C1C-C2C	-2.44	120.00	126.65
24	b	616	CLA	C11-C10-C8	-2.44	107.72	115.73
27	a	412	PL9	C37-C36-C34	-2.44	104.68	112.93
24	C	506	CLA	CHC-C1C-C2C	-2.44	120.00	126.65
24	d	405	CLA	CHC-C1C-C2C	-2.43	120.01	126.65
24	C	512	CLA	C1-C2-C3	-2.43	121.47	125.96
32	a	419	LHG	C25-C24-C23	-2.43	104.71	113.58
40	C	518	DGD	C4D-C3D-C2D	-2.43	106.55	110.84
27	A	611	PL9	C27-C28-C29	-2.43	121.58	127.68
28	l	102	SQD	C45-O47-C7	-2.42	112.16	117.88
24	B	612	CLA	O2D-CGD-O1D	-2.42	118.95	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	x	101	SQD	O8-S-O7	-2.42	105.83	111.37
26	B	619	BCR	C32-C1-C6	-2.42	106.39	110.31
40	C	518	DGD	O1G-C1A-O1A	-2.42	117.55	123.55
24	B	602	CLA	C1-C2-C3	-2.42	121.51	125.96
24	b	604	CLA	C5-C3-C2	-2.41	116.16	121.10
24	B	608	CLA	CBC-CAC-C3C	-2.41	105.58	112.41
29	B	621	LMG	O10-C28-C29	-2.41	114.17	123.68
24	b	604	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
24	C	508	CLA	CHC-C1C-C2C	-2.41	120.09	126.65
24	C	502	CLA	C16-C17-C18	-2.41	104.48	115.96
24	c	512	CLA	CBC-CAC-C3C	-2.40	105.59	112.41
24	a	407	CLA	C5-C3-C2	-2.40	116.19	121.10
24	B	606	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
28	a	424	SQD	O8-S-O7	-2.40	105.87	111.37
24	C	509	CLA	CMD-C2D-C3D	-2.40	120.44	124.89
35	d	415	P6G	O16-C17-C18	-2.40	99.08	110.15
24	a	410	CLA	O2A-CGA-O1A	-2.39	117.60	123.55
26	C	525	BCR	C15-C16-C17	-2.39	118.35	123.46
24	b	605	CLA	CHC-C1C-C2C	-2.39	120.12	126.65
24	b	604	CLA	C7-C6-C5	-2.39	106.46	113.11
24	a	408	CLA	O2A-CGA-O1A	-2.39	117.61	123.55
24	C	502	CLA	C1-C2-C3	-2.39	121.55	125.96
26	C	515	BCR	C32-C1-C6	-2.39	106.43	110.31
26	A	610	BCR	C15-C16-C17	-2.39	118.37	123.46
40	c	516	DGD	CDB-CCB-CBB	-2.39	102.16	114.45
27	A	611	PL9	C22-C21-C19	-2.39	104.86	112.93
26	C	515	BCR	C8-C7-C6	-2.38	120.58	127.25
38	b	632	HTG	C6-C5-C4	-2.38	107.43	113.00
26	c	515	BCR	C39-C30-C25	-2.38	106.44	110.31
24	a	407	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
28	x	101	SQD	O9-S-O7	-2.38	105.62	113.86
24	b	607	CLA	C1-C2-C3	-2.38	121.58	125.96
24	c	508	CLA	C4C-C3C-C2C	-2.38	103.26	106.91
26	B	620	BCR	C31-C1-C6	-2.37	106.46	110.31
24	c	502	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
31	a	401	LMT	O5'-C1'-O1'	-2.37	104.39	110.02
26	h	103	BCR	C16-C17-C18	-2.37	123.93	127.31
27	d	407	PL9	C40-C39-C38	-2.37	117.37	123.69
24	B	617	CLA	O2D-CGD-O1D	-2.37	119.06	123.82
24	b	609	CLA	C11-C12-C13	-2.37	107.97	115.73
24	C	503	CLA	OBD-CAD-C3D	-2.36	123.67	128.03
24	a	407	CLA	OBD-CAD-C3D	-2.36	123.67	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
24	c	508	CLA	O2A-CGA-O1A	-2.36	117.68	123.55
26	b	620	BCR	C1-C6-C5	-2.36	119.28	122.59
24	b	605	CLA	OBD-CAD-C3D	-2.36	123.68	128.03
24	b	611	CLA	C1-C2-C3	-2.36	121.61	125.96
26	c	527	BCR	C36-C18-C17	-2.35	119.63	122.92
29	B	634	LMG	O7-C10-O9	-2.35	117.81	123.68
24	c	504	CLA	C5-C3-C2	-2.35	116.29	121.10
24	B	611	CLA	C5-C3-C2	-2.35	116.29	121.10
28	l	102	SQD	O9-S-O7	-2.35	105.72	113.86
24	C	505	CLA	C2A-C1A-CHA	-2.35	119.76	123.92
24	C	508	CLA	C7-C6-C5	-2.35	106.59	113.11
29	C	520	LMG	O8-C28-O10	-2.35	117.72	123.55
26	a	411	BCR	C24-C23-C22	-2.35	122.69	126.21
31	t	103	LMT	O3B-C3B-C4B	-2.35	105.25	110.36
26	A	610	BCR	C15-C14-C13	-2.34	123.97	127.31
24	b	609	CLA	C5-C3-C2	-2.34	116.31	121.10
38	C	532	HTG	C4-C3-C2	-2.34	106.71	110.84
29	B	621	LMG	C1-O6-C5	-2.34	109.31	113.72
24	b	607	CLA	OBD-CAD-C3D	-2.34	123.72	128.03
24	C	504	CLA	C5-C3-C2	-2.34	116.32	121.10
26	C	525	BCR	C37-C22-C21	-2.34	119.65	122.92
24	A	606	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
26	K	101	BCR	C21-C20-C19	-2.33	116.07	123.23
38	B	630	HTG	O3-C3-C4	-2.33	105.28	110.36
27	A	611	PL9	O2-C1-C2	-2.33	116.32	121.77
24	b	615	CLA	C4C-C3C-C2C	-2.33	103.33	106.91
25	d	401	PHO	C5-C3-C2	-2.33	116.33	121.10
29	C	526	LMG	C9-C8-C7	-2.33	106.60	111.86
24	D	404	CLA	CBC-CAC-C3C	-2.33	105.80	112.41
24	b	604	CLA	OBD-CAD-C3D	-2.32	123.74	128.03
41	V	203	HEM	CMA-C3A-C4A	-2.32	124.89	128.46
24	B	603	CLA	C2A-C1A-CHA	-2.32	119.80	123.92
29	C	526	LMG	O9-C10-C11	-2.32	114.50	123.68
25	A	608	PHO	C1C-C2C-C3C	-2.32	103.82	106.51
40	C	518	DGD	O3E-C3E-C4E	-2.32	105.32	110.36
28	l	102	SQD	O8-S-O9	-2.31	106.06	111.37
26	c	527	BCR	C23-C24-C25	-2.31	120.78	127.25
28	a	413	SQD	O9-S-O7	-2.31	105.85	113.86
24	D	405	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
40	C	518	DGD	O1G-C1G-C2G	-2.31	102.85	108.66
38	H	101	HTG	C1-C2-C3	-2.31	105.75	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C15-C14-C13	-2.31	124.02	127.31
24	B	612	CLA	C1-C2-C3	-2.31	121.71	125.96
40	C	516	DGD	O3G-C3G-C2G	-2.31	105.50	110.99
24	A	607	CLA	C2A-C1A-CHA	-2.30	119.83	123.92
24	c	511	CLA	CHC-C1C-C2C	-2.30	120.37	126.65
38	H	101	HTG	C2'-C1'-S1	-2.30	104.94	112.45
24	B	610	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
26	A	610	BCR	C28-C27-C26	-2.30	109.82	113.78
24	b	602	CLA	CHC-C1C-C2C	-2.30	120.38	126.65
31	c	521	LMT	C3'-C4'-C5'	-2.30	106.00	110.88
24	A	609	CLA	O2D-CGD-O1D	-2.30	119.20	123.82
24	c	512	CLA	CBA-CAA-C2A	-2.30	106.93	113.80
26	B	618	BCR	C34-C9-C10	-2.30	119.71	122.92
24	b	614	CLA	C17-C16-C15	-2.29	102.17	113.25
24	b	602	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
24	B	609	CLA	C11-C12-C13	-2.29	108.23	115.73
24	c	510	CLA	O1D-CGD-CBD	-2.28	120.50	124.60
26	d	406	BCR	C23-C24-C25	-2.28	120.86	127.25
24	B	604	CLA	CBC-CAC-C3C	-2.28	105.93	112.41
24	B	615	CLA	CHC-C1C-C2C	-2.28	120.44	126.65
38	B	624	HTG	O2-C2-C3	-2.28	105.40	110.36
26	K	101	BCR	C23-C24-C25	-2.28	120.88	127.25
28	A	616	SQD	O47-C7-O49	-2.28	118.00	123.68
32	B	632	LHG	C6-C5-C4	-2.27	106.73	111.86
24	C	502	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
29	B	634	LMG	O2-C2-C3	-2.27	105.41	110.36
24	c	505	CLA	O2A-CGA-O1A	-2.27	117.92	123.55
25	a	409	PHO	CHD-C4C-C3C	-2.26	120.03	124.59
26	K	101	BCR	C15-C16-C17	-2.26	118.63	123.46
24	D	405	CLA	CMA-C3A-C4A	-2.26	105.69	111.77
24	B	610	CLA	C3A-C2A-C1A	-2.26	97.95	101.34
40	D	408	DGD	C1D-O6D-C5D	-2.26	109.46	113.72
40	C	516	DGD	O1G-C1G-C2G	-2.26	102.98	108.66
26	b	618	BCR	C34-C9-C10	-2.26	119.76	122.92
40	c	518	DGD	O3G-C3G-C2G	-2.26	105.62	110.99
24	d	404	CLA	C2A-C1A-CHA	-2.26	119.92	123.92
24	D	403	CLA	C2A-C1A-CHA	-2.26	119.92	123.92
24	d	404	CLA	CHC-C1C-C2C	-2.26	120.50	126.65
25	A	608	PHO	C1-C2-C3	-2.26	121.80	125.96
24	b	617	CLA	O1D-CGD-CBD	-2.25	120.55	124.60
32	B	632	LHG	O3-P-O5	-2.25	100.16	109.25
24	B	605	CLA	C2A-C1A-CHA	-2.25	119.92	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407	CLA	C2A-C1A-CHA	-2.25	119.92	123.92
28	A	612	SQD	O48-C23-O10	-2.25	117.96	123.55
24	B	607	CLA	O2A-CGA-O1A	-2.25	117.96	123.55
26	d	406	BCR	C10-C11-C12	-2.25	116.33	123.23
26	D	406	BCR	C15-C16-C17	-2.25	118.67	123.46
24	b	614	CLA	O2A-CGA-O1A	-2.25	117.97	123.55
30	C	528	GOL	O1-C1-C2	-2.24	98.76	110.07
31	A	617	LMT	O2B-C2B-C3B	-2.24	105.48	110.36
24	C	510	CLA	CHC-C1C-C2C	-2.24	120.53	126.65
24	b	611	CLA	CHC-C1C-C2C	-2.24	120.54	126.65
24	c	501	CLA	C4C-C3C-C2C	-2.24	103.47	106.91
24	b	605	CLA	C2A-C1A-CHA	-2.24	119.95	123.92
24	c	503	CLA	CHC-C1C-C2C	-2.24	120.55	126.65
26	B	620	BCR	C20-C21-C22	-2.24	124.12	127.31
24	C	504	CLA	O2D-CGD-O1D	-2.23	119.33	123.82
24	B	612	CLA	C11-C12-C13	-2.23	108.40	115.73
24	B	617	CLA	CHC-C1C-C2C	-2.23	120.57	126.65
28	l	102	SQD	O47-C7-O49	-2.23	118.12	123.68
27	d	407	PL9	C36-C37-C38	-2.23	104.33	111.97
27	A	611	PL9	C21-C19-C18	-2.22	116.55	121.10
24	C	512	CLA	O2D-CGD-O1D	-2.22	119.35	123.82
24	B	610	CLA	CHC-C1C-C2C	-2.22	120.59	126.65
32	D	411	LHG	O8-C23-O10	-2.22	118.03	123.55
26	B	620	BCR	C11-C10-C9	-2.22	124.14	127.31
24	B	607	CLA	CHC-C1C-C2C	-2.22	120.60	126.65
26	c	515	BCR	C15-C16-C17	-2.22	118.73	123.46
24	d	404	CLA	C5-C3-C2	-2.22	116.56	121.10
24	c	502	CLA	C2A-C1A-CHA	-2.21	119.99	123.92
26	t	102	BCR	C19-C18-C17	-2.21	115.55	118.94
24	c	513	CLA	C4C-C3C-C2C	-2.21	103.52	106.91
24	b	616	CLA	OBD-CAD-C3D	-2.21	123.95	128.03
32	B	632	LHG	O8-C23-O10	-2.21	118.06	123.55
40	H	103	DGD	C1D-O6D-C5D	-2.21	109.55	113.72
24	b	606	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	c	508	CLA	CHC-C1C-C2C	-2.21	120.63	126.65
24	B	602	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
28	a	424	SQD	O47-C7-O49	-2.21	118.17	123.68
31	c	521	LMT	O5'-C1'-O1'	-2.20	104.79	110.02
24	c	509	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
24	c	509	CLA	O2D-CGD-O1D	-2.20	119.39	123.82
24	c	503	CLA	C7-C6-C5	-2.20	107.00	113.11
24	c	511	CLA	C5-C3-C2	-2.20	116.60	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C2A-C1A-CHA	-2.19	120.03	123.92
26	D	406	BCR	C10-C11-C12	-2.19	116.51	123.23
40	c	518	DGD	C6B-C5B-C4B	-2.19	103.18	114.45
28	A	622	SQD	O6-C44-C45	-2.19	105.79	110.99
24	a	410	CLA	CHC-C1C-C2C	-2.18	120.69	126.65
24	D	403	CLA	C4C-C3C-C2C	-2.18	103.56	106.91
24	B	608	CLA	CHC-C1C-C2C	-2.18	120.70	126.65
24	B	611	CLA	CAA-CBA-CGA	-2.18	106.78	113.35
24	b	604	CLA	CBC-CAC-C3C	-2.18	106.22	112.41
28	F	104	SQD	C1-O5-C5	-2.18	109.61	113.72
24	b	611	CLA	C20-C18-C19	-2.18	100.19	110.50
27	D	407	PL9	C22-C23-C24	-2.18	122.21	127.68
27	a	412	PL9	C22-C21-C19	-2.18	105.56	112.93
31	a	401	LMT	C1'-C2'-C3'	-2.18	105.94	109.98
26	c	514	BCR	C12-C13-C14	-2.17	115.61	118.94
24	B	605	CLA	C4C-C3C-C2C	-2.17	103.58	106.91
29	c	519	LMG	C6-C5-C4	-2.17	107.92	113.00
24	b	613	CLA	C11-C12-C13	-2.17	108.61	115.73
24	A	606	CLA	CHD-C4C-C3C	-2.17	121.65	124.92
24	b	602	CLA	O1D-CGD-CBD	-2.17	120.71	124.60
26	A	610	BCR	C23-C24-C25	-2.17	121.19	127.25
26	c	514	BCR	C38-C26-C25	-2.16	122.08	124.51
24	b	608	CLA	C1C-C2C-C3C	-2.16	104.52	106.92
24	c	510	CLA	O2D-CGD-O1D	-2.16	119.47	123.82
32	E	101	LHG	O8-C23-O10	-2.16	118.19	123.55
32	a	419	LHG	O7-C7-O9	-2.16	118.29	123.68
24	c	507	CLA	OBD-CAD-C3D	-2.16	124.05	128.03
24	b	609	CLA	CHC-C1C-C2C	-2.16	120.77	126.65
24	a	407	CLA	CAA-CBA-CGA	-2.16	106.85	113.35
24	B	609	CLA	CHC-C1C-C2C	-2.16	120.77	126.65
26	b	619	BCR	C24-C23-C22	-2.15	122.98	126.21
24	B	603	CLA	C1C-C2C-C3C	-2.15	104.53	106.92
32	E	101	LHG	O7-C7-O9	-2.15	118.31	123.68
26	B	619	BCR	C15-C16-C17	-2.15	118.87	123.46
24	b	602	CLA	C4-C3-C2	-2.15	117.97	123.69
26	c	514	BCR	C15-C14-C13	-2.15	124.25	127.31
24	B	608	CLA	OBD-CAD-C3D	-2.14	124.07	128.03
24	B	615	CLA	OBD-CAD-C3D	-2.14	124.08	128.03
26	K	101	BCR	C10-C11-C12	-2.14	116.66	123.23
38	c	531	HTG	C4-C3-C2	-2.14	107.06	110.84
25	D	401	PHO	CHD-C4C-C3C	-2.14	120.28	124.59
24	b	614	CLA	C2A-C1A-CHA	-2.14	120.12	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	O2D-CGD-O1D	-2.14	119.52	123.82
24	c	511	CLA	C11-C10-C8	-2.14	108.72	115.73
26	T	102	BCR	C15-C16-C17	-2.14	118.90	123.46
24	C	513	CLA	C1C-C2C-C3C	-2.14	104.55	106.92
28	A	612	SQD	C5-C6-S	-2.13	111.37	114.34
26	A	610	BCR	C37-C22-C21	-2.13	119.94	122.92
24	C	512	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
31	f	101	LMT	C6'-C5'-C4'	-2.13	107.43	113.24
24	b	603	CLA	C1C-C2C-C3C	-2.13	104.56	106.92
24	c	509	CLA	C15-C13-C12	-2.12	101.89	112.10
24	c	510	CLA	O2A-CGA-O1A	-2.12	118.28	123.55
24	c	506	CLA	O2A-CGA-O1A	-2.12	118.28	123.55
24	B	614	CLA	CMD-C2D-C3D	-2.12	120.95	124.89
38	C	530	HTG	O4-C4-C3	-2.12	105.74	110.36
28	A	616	SQD	C1-C2-C3	-2.12	106.03	109.98
32	D	411	LHG	O7-C7-O9	-2.12	118.38	123.68
24	b	613	CLA	O2D-CGD-O1D	-2.12	119.55	123.82
24	C	503	CLA	O2A-CGA-O1A	-2.12	118.29	123.55
24	b	604	CLA	O2A-CGA-O1A	-2.12	118.29	123.55
26	T	102	BCR	C7-C6-C5	-2.12	116.49	121.54
24	b	605	CLA	O1D-CGD-CBD	-2.12	120.80	124.60
26	C	515	BCR	C4-C5-C6	-2.12	119.63	122.74
26	c	514	BCR	C8-C7-C6	-2.12	121.33	127.25
40	H	103	DGD	C3D-C4D-C5D	-2.12	106.49	110.22
28	x	101	SQD	O48-C23-O10	-2.12	118.30	123.55
24	B	610	CLA	CBC-CAC-C3C	-2.11	106.41	112.41
26	D	406	BCR	C8-C7-C6	-2.11	121.33	127.25
24	C	510	CLA	O1D-CGD-CBD	-2.11	120.81	124.60
24	C	504	CLA	CBC-CAC-C3C	-2.11	106.42	112.41
24	C	504	CLA	CHD-C4C-C3C	-2.11	121.74	124.92
24	B	604	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
25	D	401	PHO	C1C-C2C-C3C	-2.11	104.07	106.51
24	D	404	CLA	C4C-C3C-C2C	-2.11	103.68	106.91
24	c	506	CLA	CHC-C1C-C2C	-2.11	120.91	126.65
26	K	101	BCR	C36-C18-C17	-2.10	119.98	122.92
29	b	621	LMG	O8-C9-C8	-2.10	103.38	108.66
26	b	619	BCR	C7-C8-C9	-2.10	123.06	126.21
24	b	612	CLA	C4C-C3C-C2C	-2.10	103.69	106.91
32	d	409	LHG	C11-C10-C9	-2.09	103.69	114.45
40	C	516	DGD	CDB-CCB-CBB	-2.09	103.69	114.45
32	e	101	LHG	O8-C23-O10	-2.09	118.37	123.55
25	A	608	PHO	CBA-CAA-C2A	-2.09	107.55	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	v	202	HEM	C3C-C4C-NC	-2.09	107.00	110.94
29	C	526	LMG	C1-O6-C5	-2.08	109.79	113.72
24	c	508	CLA	C2A-C1A-CHA	-2.08	120.23	123.92
24	b	609	CLA	C6-C7-C8	-2.08	108.90	115.73
24	c	504	CLA	OBD-CAD-C3D	-2.08	124.19	128.03
24	d	403	CLA	C1C-C2C-C3C	-2.08	104.61	106.92
24	A	609	CLA	CHC-C1C-C2C	-2.08	120.98	126.65
26	C	525	BCR	C33-C5-C6	-2.08	122.18	124.51
26	d	406	BCR	C15-C16-C17	-2.08	119.03	123.46
24	b	616	CLA	CHC-C1C-C2C	-2.08	120.98	126.65
24	C	509	CLA	C16-C17-C18	-2.08	106.05	115.96
28	x	101	SQD	C1-C2-C3	-2.08	106.12	109.98
32	B	632	LHG	C9-C8-C7	-2.07	106.01	113.58
24	C	501	CLA	C4C-C3C-C2C	-2.07	103.73	106.91
26	h	103	BCR	C36-C18-C17	-2.07	120.02	122.92
38	B	630	HTG	O5-C1-C2	-2.07	107.44	110.28
38	O	303	HTG	O5-C1-C2	-2.07	107.44	110.28
24	B	605	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
26	b	619	BCR	C11-C10-C9	-2.07	124.36	127.31
29	B	621	LMG	O5-C6-C5	-2.06	104.39	111.34
24	c	508	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
24	c	507	CLA	CBC-CAC-C3C	-2.06	106.55	112.41
32	e	101	LHG	O7-C7-O9	-2.06	118.53	123.68
40	c	518	DGD	O1G-C1A-O1A	-2.06	118.43	123.55
24	b	603	CLA	C16-C17-C18	-2.06	106.12	115.96
26	k	101	BCR	C21-C20-C19	-2.06	116.91	123.23
24	B	606	CLA	O2A-CGA-O1A	-2.06	118.44	123.55
29	c	520	LMG	O8-C28-O10	-2.06	118.44	123.55
26	a	411	BCR	C39-C30-C25	-2.06	106.97	110.31
26	c	527	BCR	C15-C16-C17	-2.05	119.08	123.46
24	B	614	CLA	C7-C6-C5	-2.05	107.41	113.11
24	c	511	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
26	c	515	BCR	C20-C19-C18	-2.05	120.66	126.42
40	C	516	DGD	O1G-C1A-O1A	-2.05	118.46	123.55
24	C	504	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
24	C	512	CLA	C17-C16-C15	-2.05	103.34	113.25
24	b	610	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
30	D	402	GOL	O2-C2-C1	-2.05	99.17	108.84
24	B	605	CLA	CHC-C1C-C2C	-2.05	121.07	126.65
24	B	602	CLA	O1D-CGD-CBD	-2.04	120.93	124.60
24	b	615	CLA	OBD-CAD-C3D	-2.04	124.26	128.03
28	A	616	SQD	C5-C6-S	-2.04	111.49	114.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	C6-C7-C8	-2.04	109.03	115.73
24	C	511	CLA	O2A-CGA-O1A	-2.04	118.49	123.55
31	j	103	LMT	O4'-C4B-C3B	-2.04	105.92	110.36
28	A	612	SQD	C45-O47-C7	-2.04	113.06	117.88
29	b	621	LMG	C4-C3-C2	-2.04	107.24	110.84
26	k	101	BCR	C1-C6-C5	-2.04	119.73	122.59
28	F	104	SQD	O48-C23-O10	-2.03	118.50	123.55
32	d	409	LHG	C27-C26-C25	-2.03	103.98	114.45
24	c	504	CLA	C6-C7-C8	-2.03	109.07	115.73
25	D	401	PHO	CHC-C1C-C2C	-2.03	120.97	125.62
26	d	406	BCR	C34-C9-C10	-2.03	120.08	122.92
27	a	412	PL9	C36-C34-C33	-2.03	116.95	121.10
41	v	202	HEM	CBA-CAA-C2A	-2.03	108.61	112.48
28	x	101	SQD	O47-C7-O49	-2.03	118.62	123.68
29	C	519	LMG	C1-O6-C5	-2.02	109.90	113.72
24	C	511	CLA	CHC-C1C-C2C	-2.02	121.13	126.65
24	d	405	CLA	CGD-CBD-CAD	-2.02	103.94	110.71
24	b	612	CLA	C7-C6-C5	-2.02	107.50	113.11
26	t	102	BCR	C32-C1-C6	-2.02	107.04	110.31
24	B	606	CLA	C1C-C2C-C3C	-2.01	104.69	106.92
24	B	612	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
24	b	609	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
24	B	613	CLA	C1C-C2C-C3C	-2.01	104.69	106.92
24	A	606	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
28	h	105	SQD	O6-C44-C45	-2.01	106.20	110.99
24	c	507	CLA	CHC-C1C-C2C	-2.01	121.17	126.65
31	a	401	LMT	O1B-C4'-C5'	-2.01	104.40	109.34
26	C	525	BCR	C11-C10-C9	-2.01	124.44	127.31
24	B	616	CLA	C9-C8-C7	-2.01	104.03	111.36
24	B	611	CLA	C3A-C2A-C1A	-2.01	98.33	101.34
24	c	503	CLA	CBC-CAC-C3C	-2.01	106.72	112.41
24	C	512	CLA	C1C-C2C-C3C	-2.01	104.70	106.92
28	h	105	SQD	O3-C3-C2	-2.01	105.99	110.36
24	D	404	CLA	O2A-CGA-O1A	-2.00	118.57	123.55
25	a	409	PHO	CAA-CBA-CGA	-2.00	107.31	113.35
26	D	406	BCR	C21-C20-C19	-2.00	117.08	123.23
24	C	505	CLA	O2A-CGA-O1A	-2.00	118.58	123.55
28	A	616	SQD	C4-C3-C2	-2.00	107.31	110.84
24	c	503	CLA	CAC-C3C-C4C	2.00	127.65	124.83
24	C	503	CLA	CHB-C4A-NA	2.00	127.28	124.51
26	d	406	BCR	C2-C1-C6	2.00	113.61	110.48
28	l	102	SQD	C3-C4-C5	2.00	113.75	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	622	LMT	O3B-C3B-C4B	2.01	114.72	110.36
24	c	511	CLA	C4-C3-C5	2.01	118.77	115.29
29	B	634	LMG	O7-C8-C9	2.01	115.73	108.44
24	B	610	CLA	C1D-CHD-C4C	2.01	125.23	122.48
38	a	418	HTG	O5-C5-C4	2.01	113.37	109.66
31	m	101	LMT	C2'-C3'-C4'	2.01	113.78	109.61
24	A	606	CLA	CMD-C2D-C3D	2.01	128.63	124.89
31	Y	101	LMT	C4B-C3B-C2B	2.02	114.39	110.84
24	c	508	CLA	C1D-CHD-C4C	2.02	125.24	122.48
24	B	604	CLA	CED-O2D-CGD	2.02	120.71	115.97
24	a	408	CLA	CED-O2D-CGD	2.02	120.71	115.97
24	b	615	CLA	C20-C18-C19	2.02	120.07	110.50
31	j	103	LMT	O5'-C5'-C4'	2.02	113.89	109.75
27	A	611	PL9	C25-C24-C26	2.03	118.80	115.29
40	H	103	DGD	C6D-C5D-C4D	2.03	116.32	112.00
24	b	607	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	B	606	CLA	CMB-C2B-C3B	2.03	128.67	124.89
29	C	519	LMG	O6-C5-C6	2.04	111.28	106.41
24	b	606	CLA	C1D-CHD-C4C	2.04	125.27	122.48
24	c	506	CLA	C3D-CAD-CBD	2.04	110.48	107.60
31	Y	101	LMT	O2B-C2B-C1B	2.04	114.30	110.03
24	b	602	CLA	CMB-C2B-C1B	2.04	131.60	128.46
26	C	514	BCR	C32-C1-C31	2.04	114.76	108.50
26	K	101	BCR	C34-C9-C10	2.04	125.78	122.92
24	d	403	CLA	CHB-C4A-NA	2.04	127.34	124.51
31	C	533	LMT	C1'-O5'-C5'	2.05	117.57	113.72
24	c	505	CLA	O2A-CGA-CBA	2.05	117.85	111.90
25	a	409	PHO	CAC-C3C-C2C	2.05	131.04	127.49
32	D	411	LHG	O7-C7-C8	2.05	115.81	111.55
38	b	632	HTG	C1-C2-C3	2.05	115.08	110.69
40	C	516	DGD	O4E-C4E-C3E	2.05	114.83	110.36
31	b	622	LMT	C1B-C2B-C3B	2.06	113.80	109.98
24	a	408	CLA	CMB-C2B-C3B	2.06	128.71	124.89
31	m	101	LMT	O1'-C1'-C2'	2.06	111.59	108.23
32	E	101	LHG	O8-C23-C24	2.06	117.89	111.90
38	c	523	HTG	C3-C4-C5	2.06	113.85	110.22
38	B	630	HTG	O4-C4-C5	2.06	114.48	109.28
24	C	501	CLA	CHB-C4A-NA	2.07	127.37	124.51
24	c	501	CLA	CAC-C3C-C4C	2.07	127.74	124.83
38	C	531	HTG	O2-C2-C1	2.07	114.39	110.27
27	D	407	PL9	C20-C19-C21	2.07	118.88	115.29
38	c	522	HTG	O5-C5-C6	2.07	111.37	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	C	532	HTG	C1'-S1-C1	2.07	103.35	100.28
24	c	511	CLA	C1-O2A-CGA	2.07	121.74	116.77
38	b	623	HTG	C1-O5-C5	2.08	116.69	112.69
24	c	504	CLA	CAC-C3C-C4C	2.08	127.76	124.83
24	C	511	CLA	C3A-C2A-C1A	2.08	104.45	101.34
24	b	607	CLA	CAA-C2A-C1A	2.08	118.79	111.97
26	D	406	BCR	C3-C4-C5	2.08	117.36	113.78
31	m	101	LMT	C3B-C4B-C5B	2.08	113.89	110.22
24	c	506	CLA	CMB-C2B-C3B	2.08	128.76	124.89
31	c	521	LMT	O6B-C6B-C5B	2.08	118.35	111.34
25	A	608	PHO	CMC-C2C-C1C	2.08	128.29	125.04
26	A	610	BCR	C35-C13-C14	2.09	125.84	122.92
40	H	103	DGD	O1G-C1A-C2A	2.09	117.97	111.90
31	Y	101	LMT	C1B-O1B-C4'	2.09	123.08	118.00
24	C	505	CLA	C6-C5-C3	2.09	117.39	112.66
38	B	630	HTG	C1-O5-C5	2.09	116.72	112.69
31	J	103	LMT	O1B-C1B-O5B	2.09	115.78	110.70
24	C	506	CLA	CHB-C4A-NA	2.10	127.41	124.51
35	I	106	P6G	C17-O16-C15	2.10	122.38	113.30
28	x	101	SQD	O3-C3-C2	2.10	114.92	110.36
24	B	613	CLA	O2A-CGA-CBA	2.10	118.01	111.90
24	d	404	CLA	CED-O2D-CGD	2.10	120.89	115.97
26	k	101	BCR	C1-C6-C7	2.10	121.63	115.73
24	A	609	CLA	CMB-C2B-C3B	2.10	128.79	124.89
25	a	409	PHO	C2B-C1B-NB	2.10	112.93	109.82
31	I	101	LMT	C4B-C3B-C2B	2.11	114.55	110.84
38	H	101	HTG	O2-C2-C1	2.11	114.47	110.27
24	b	617	CLA	CHB-C4A-NA	2.11	127.43	124.51
24	B	602	CLA	C1-O2A-CGA	2.11	121.83	116.77
28	a	424	SQD	C45-O47-C7	2.11	122.86	117.88
31	B	622	LMT	O5B-C5B-C6B	2.11	111.46	106.41
27	D	407	PL9	C2-C1-C6	2.11	121.36	117.82
24	c	509	CLA	CMB-C2B-C3B	2.11	128.81	124.89
24	B	602	CLA	C7-C6-C5	2.11	118.98	113.11
29	z	101	LMG	O8-C28-C29	2.11	118.05	111.90
30	b	625	GOL	O2-C2-C1	2.11	118.82	108.84
24	d	403	CLA	CMB-C2B-C3B	2.12	128.82	124.89
25	D	401	PHO	CMC-C2C-C1C	2.12	128.34	125.04
24	b	611	CLA	O2A-CGA-CBA	2.12	118.07	111.90
38	C	532	HTG	O2-C2-C1	2.12	114.50	110.27
24	B	603	CLA	CAC-C3C-C2C	2.12	131.17	127.49
24	B	615	CLA	C4-C3-C5	2.12	118.97	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	533	LMT	O1B-C1B-C2B	2.13	112.90	108.11
24	c	506	CLA	C16-C17-C18	2.13	126.11	115.96
27	A	611	PL9	C8-C7-C3	2.13	118.02	111.73
38	B	631	HTG	O5-C1-S1	2.13	115.79	110.15
31	c	521	LMT	C1'-O5'-C5'	2.13	117.73	113.72
26	b	618	BCR	C35-C13-C12	2.13	121.49	118.10
38	C	522	HTG	O5-C5-C4	2.13	113.58	109.66
24	d	403	CLA	CAC-C3C-C4C	2.13	127.84	124.83
31	I	101	LMT	O6B-C6B-C5B	2.13	118.52	111.34
26	D	406	BCR	C24-C25-C26	2.14	126.63	121.54
39	V	217	1PE	OH3-C22-C12	2.14	120.03	110.15
40	H	103	DGD	O2G-C1B-C2B	2.14	116.00	111.55
34	O	309	PGE	C5-O3-C4	2.14	122.59	113.30
29	c	519	LMG	O8-C9-C8	2.15	114.05	108.66
28	A	616	SQD	O2-C2-C3	2.15	115.03	110.36
24	B	617	CLA	C6-C5-C3	2.15	117.52	112.66
26	d	406	BCR	C4-C5-C6	2.15	125.90	122.74
40	H	103	DGD	C6E-C5E-C4E	2.15	118.03	113.00
26	c	514	BCR	C36-C18-C19	2.15	121.53	118.10
24	b	612	CLA	CHB-C4A-NA	2.15	127.49	124.51
24	c	505	CLA	O2D-CGD-CBD	2.16	115.15	111.30
25	a	409	PHO	C4A-NA-C1A	2.16	109.91	108.16
24	c	508	CLA	CMC-C2C-C1C	2.16	128.29	125.02
24	c	508	CLA	CHB-C4A-NA	2.16	127.50	124.51
28	F	104	SQD	O2-C2-C3	2.16	115.05	110.36
30	B	625	GOL	O2-C2-C1	2.16	119.05	108.84
30	t	101	GOL	C3-C2-C1	2.16	120.12	111.52
24	c	501	CLA	O1D-CGD-CBD	2.17	128.49	124.60
24	B	617	CLA	C5-C3-C2	2.17	125.54	121.10
40	h	104	DGD	C6D-C5D-C4D	2.17	116.62	112.00
31	a	401	LMT	O2B-C2B-C1B	2.17	114.57	110.03
24	C	511	CLA	CED-O2D-CGD	2.17	121.06	115.97
24	D	403	CLA	CMB-C2B-C3B	2.17	128.92	124.89
24	b	602	CLA	C6-C5-C3	2.17	117.58	112.66
24	c	507	CLA	CMB-C2B-C3B	2.17	128.93	124.89
40	D	408	DGD	O1G-C1G-C2G	2.18	114.12	108.66
24	b	607	CLA	C1-O2A-CGA	2.18	121.99	116.77
24	B	605	CLA	C1D-CHD-C4C	2.18	125.46	122.48
31	m	102	LMT	O5'-C5'-C6'	2.18	111.64	106.41
24	b	605	CLA	C3D-CAD-CBD	2.18	110.68	107.60
26	H	102	BCR	C15-C14-C13	2.19	130.43	127.31
26	c	527	BCR	C29-C30-C25	2.19	113.89	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	411	LHG	O7-C7-C8	2.19	116.09	111.55
24	c	507	CLA	C4-C3-C5	2.19	119.08	115.29
26	c	515	BCR	C36-C18-C19	2.19	121.58	118.10
31	j	103	LMT	O1B-C4'-C3'	2.19	112.47	107.19
24	A	606	CLA	CMC-C2C-C1C	2.19	128.35	125.02
24	B	606	CLA	O2D-CGD-CBD	2.20	115.22	111.30
30	a	415	GOL	O1-C1-C2	2.20	121.15	110.07
38	h	101	HTG	C1-O5-C5	2.20	116.93	112.69
27	a	412	PL9	C20-C19-C21	2.20	119.11	115.29
24	D	404	CLA	CED-O2D-CGD	2.20	121.14	115.97
25	a	409	PHO	C2D-C1D-ND	2.20	113.08	109.82
24	b	614	CLA	CMB-C2B-C3B	2.20	128.98	124.89
38	b	631	HTG	C1-O5-C5	2.20	116.94	112.69
38	b	631	HTG	O5-C1-S1	2.21	116.00	110.15
40	c	518	DGD	O6D-C1D-C2D	2.21	114.56	110.30
29	B	634	LMG	C1-C2-C3	2.21	114.09	109.98
24	b	615	CLA	C1-O2A-CGA	2.21	122.08	116.77
24	b	617	CLA	CMC-C2C-C1C	2.21	128.38	125.02
24	B	605	CLA	CMC-C2C-C1C	2.22	128.38	125.02
31	t	103	LMT	O1B-C1B-O5B	2.22	116.08	110.70
29	c	519	LMG	C7-O1-C1	2.22	118.31	113.76
24	c	508	CLA	CMB-C2B-C3B	2.22	129.01	124.89
24	C	513	CLA	CED-O2D-CGD	2.22	121.17	115.97
38	c	531	HTG	O5-C5-C6	2.22	111.73	106.41
30	B	628	GOL	C3-C2-C1	2.22	120.34	111.52
30	b	627	GOL	O3-C3-C2	2.22	121.27	110.07
24	C	508	CLA	CMC-C2C-C1C	2.22	128.39	125.02
24	B	605	CLA	CED-O2D-CGD	2.22	121.18	115.97
24	C	501	CLA	CMB-C2B-C3B	2.23	129.02	124.89
40	c	517	DGD	O5D-C6D-C5D	2.23	112.67	108.94
29	z	101	LMG	O1-C1-C2	2.23	111.87	108.23
24	b	613	CLA	O2A-CGA-CBA	2.24	118.41	111.90
38	V	204	HTG	O4-C4-C3	2.24	115.23	110.36
32	a	419	LHG	O8-C23-C24	2.25	118.43	111.90
29	B	634	LMG	C1-O6-C5	2.25	117.94	113.72
24	B	603	CLA	CAC-C3C-C4C	2.25	128.00	124.83
24	C	511	CLA	CMB-C2B-C3B	2.25	129.07	124.89
41	E	113	HEM	CMB-C2B-C3B	2.25	129.07	124.89
41	E	113	HEM	CMD-C2D-C1D	2.25	131.93	128.46
24	c	505	CLA	C1D-CHD-C4C	2.25	125.56	122.48
26	C	514	BCR	C37-C22-C23	2.25	121.69	118.10
27	d	407	PL9	C51-C49-C48	2.25	129.45	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	602	CLA	C4-C3-C5	2.26	119.20	115.29
26	k	101	BCR	C34-C9-C10	2.26	126.08	122.92
24	B	607	CLA	CED-O2D-CGD	2.26	121.26	115.97
26	B	618	BCR	C8-C9-C10	2.26	122.41	118.94
38	b	632	HTG	O5-C1-C2	2.26	113.38	110.28
26	t	102	BCR	C1-C6-C7	2.27	122.10	115.73
26	C	514	BCR	C29-C30-C25	2.27	114.02	110.48
24	A	606	CLA	CHB-C4A-NA	2.28	127.66	124.51
24	c	513	CLA	O2D-CGD-CBD	2.28	115.37	111.30
26	b	619	BCR	C24-C25-C26	2.28	126.97	121.54
24	B	609	CLA	CAC-C3C-C4C	2.28	128.05	124.83
31	m	101	LMT	C1-O1'-C1'	2.28	117.79	113.87
28	A	622	SQD	O8-S-C6	2.29	108.81	106.01
38	c	531	HTG	O3-C3-C2	2.29	115.34	110.36
24	B	611	CLA	O2A-CGA-CBA	2.29	118.56	111.90
27	d	407	PL9	C7-C3-C4	2.29	118.74	116.88
38	V	204	HTG	O5-C5-C6	2.29	111.90	106.41
26	h	103	BCR	C28-C27-C26	2.29	117.73	113.78
24	b	610	CLA	CMC-C2C-C1C	2.30	128.50	125.02
26	C	515	BCR	C2-C1-C6	2.30	114.07	110.48
40	c	518	DGD	O1G-C1A-C2A	2.30	118.58	111.90
24	c	510	CLA	CMC-C2C-C1C	2.30	128.50	125.02
26	t	102	BCR	C40-C30-C25	2.30	114.04	110.31
27	a	412	PL9	C15-C14-C16	2.30	119.28	115.29
38	b	623	HTG	C1-C2-C3	2.30	115.62	110.69
26	T	102	BCR	C31-C1-C6	2.31	114.05	110.31
29	d	412	LMG	O1-C1-C2	2.31	112.00	108.23
28	A	612	SQD	O3-C3-C4	2.31	115.38	110.36
29	c	520	LMG	C9-O8-C28	2.31	124.08	117.13
26	b	619	BCR	C34-C9-C10	2.31	126.16	122.92
28	b	633	SQD	O4-C4-C3	2.31	115.38	110.36
24	B	604	CLA	CAC-C3C-C4C	2.31	128.09	124.83
40	d	408	DGD	C4D-C3D-C2D	2.31	114.92	110.84
31	m	101	LMT	O1B-C1B-C2B	2.31	113.32	108.11
24	c	505	CLA	CAA-C2A-C1A	2.31	119.56	111.97
24	C	511	CLA	C1-O2A-CGA	2.32	122.33	116.77
24	B	605	CLA	CHB-C4A-NA	2.32	127.71	124.51
26	c	514	BCR	C32-C1-C6	2.32	114.06	110.31
24	b	607	CLA	C2A-C3A-C4A	2.32	105.61	101.87
28	a	417	SQD	O6-C1-C2	2.32	112.02	108.23
29	d	412	LMG	O6-C5-C4	2.32	113.93	109.66
24	c	506	CLA	O1D-CGD-CBD	2.32	128.77	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	519	LMG	C3-C4-C5	2.32	114.30	110.22
24	B	610	CLA	C6-C5-C3	2.32	117.92	112.66
25	d	401	PHO	CED-O2D-CGD	2.32	121.42	115.97
24	D	403	CLA	CMC-C2C-C1C	2.32	128.54	125.02
24	C	512	CLA	O2A-CGA-CBA	2.33	118.67	111.90
28	a	417	SQD	O9-S-C6	2.33	108.82	106.83
24	C	510	CLA	O2D-CGD-CBD	2.33	115.47	111.30
28	F	104	SQD	O47-C7-C8	2.34	116.40	111.55
31	t	103	LMT	O1B-C4'-C3'	2.34	112.81	107.19
38	b	631	HTG	O4-C4-C5	2.34	115.17	109.28
24	b	607	CLA	C3D-CAD-CBD	2.34	110.90	107.60
24	C	502	CLA	CHB-C4A-NA	2.34	127.75	124.51
31	M	101	LMT	O5B-C5B-C4B	2.34	113.97	109.66
28	b	633	SQD	O8-S-C6	2.34	108.87	106.01
24	c	510	CLA	CMB-C2B-C3B	2.35	129.25	124.89
28	b	633	SQD	O2-C2-C1	2.35	114.94	110.03
31	M	101	LMT	C2'-C3'-C4'	2.35	114.48	109.61
28	a	413	SQD	O2-C2-C1	2.35	114.94	110.03
24	b	615	CLA	CMB-C2B-C3B	2.35	129.25	124.89
24	b	617	CLA	C1-O2A-CGA	2.35	122.42	116.77
24	a	410	CLA	CMB-C2B-C3B	2.36	129.26	124.89
27	D	407	PL9	C53-C6-C1	2.36	119.85	114.84
24	b	606	CLA	CMB-C2B-C1B	2.36	132.09	128.46
27	a	412	PL9	C7-C8-C9	2.36	130.66	126.71
24	B	613	CLA	CMC-C2C-C1C	2.36	128.60	125.02
31	c	521	LMT	O4'-C4B-C3B	2.36	115.50	110.36
24	C	512	CLA	CMB-C2B-C3B	2.36	129.28	124.89
38	C	521	HTG	C1'-S1-C1	2.37	103.79	100.28
38	a	418	HTG	O2-C2-C1	2.37	114.98	110.27
24	B	610	CLA	CED-O2D-CGD	2.37	121.52	115.97
26	T	102	BCR	C36-C18-C19	2.38	121.88	118.10
24	C	508	CLA	C1D-CHD-C4C	2.38	125.73	122.48
29	C	520	LMG	O6-C5-C6	2.38	112.11	106.41
28	A	622	SQD	O47-C7-C8	2.38	116.49	111.55
28	b	633	SQD	O6-C44-C45	2.38	116.66	110.99
24	b	617	CLA	CED-O2D-CGD	2.38	121.56	115.97
31	c	521	LMT	O5'-C1'-C2'	2.39	114.90	110.30
24	C	506	CLA	C3D-CAD-CBD	2.39	110.98	107.60
29	C	526	LMG	O8-C28-C29	2.39	118.87	111.90
25	D	401	PHO	C4A-NA-C1A	2.40	110.10	108.16
24	a	410	CLA	O2D-CGD-CBD	2.40	115.58	111.30
31	I	101	LMT	C1B-O5B-C5B	2.40	118.24	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	413	SQD	C46-C45-C44	2.40	117.28	111.86
24	c	512	CLA	CAC-C3C-C4C	2.41	128.23	124.83
31	t	103	LMT	C1-O1'-C1'	2.41	118.00	113.87
38	B	630	HTG	O2-C2-C3	2.41	115.60	110.36
29	C	520	LMG	O4-C4-C5	2.41	115.36	109.28
24	c	506	CLA	CAC-C3C-C4C	2.41	128.24	124.83
24	c	503	CLA	CED-O2D-CGD	2.42	121.63	115.97
24	C	506	CLA	C1-O2A-CGA	2.42	122.57	116.77
26	B	620	BCR	C2-C1-C6	2.42	114.26	110.48
29	J	101	LMG	O6-C1-C2	2.43	114.97	110.30
24	b	609	CLA	CAC-C3C-C4C	2.43	128.25	124.83
28	b	633	SQD	O2-C2-C3	2.43	115.64	110.36
24	B	602	CLA	C11-C10-C8	2.43	123.72	115.73
24	C	506	CLA	CMB-C2B-C3B	2.43	129.41	124.89
24	B	608	CLA	O2D-CGD-CBD	2.44	115.65	111.30
24	C	502	CLA	CMB-C2B-C3B	2.44	129.42	124.89
28	x	101	SQD	C46-O48-C23	2.44	124.47	117.13
24	C	513	CLA	CMC-C2C-C1C	2.44	128.72	125.02
31	u	203	LMT	O2'-C2'-C1'	2.44	115.13	110.03
24	b	612	CLA	C3D-CAD-CBD	2.44	111.05	107.60
24	C	509	CLA	CMB-C2B-C3B	2.44	129.43	124.89
25	a	409	PHO	CED-O2D-CGD	2.44	121.70	115.97
29	C	526	LMG	C3-C4-C5	2.45	114.53	110.22
38	c	531	HTG	O2-C2-C3	2.45	115.69	110.36
24	C	510	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	B	607	CLA	C3D-CAD-CBD	2.45	111.06	107.60
24	C	507	CLA	O2A-CGA-CBA	2.45	119.03	111.90
24	b	610	CLA	CED-O2D-CGD	2.45	121.72	115.97
24	b	602	CLA	O2A-CGA-CBA	2.46	119.05	111.90
31	B	622	LMT	O1B-C4'-C3'	2.46	113.11	107.19
24	b	613	CLA	CED-O2D-CGD	2.46	121.73	115.97
24	B	608	CLA	CAC-C3C-C4C	2.46	128.30	124.83
26	B	618	BCR	C37-C22-C23	2.46	122.02	118.10
32	a	419	LHG	C6-O8-C23	2.46	124.54	117.13
24	C	503	CLA	C3D-CAD-CBD	2.48	111.10	107.60
31	u	203	LMT	O2B-C2B-C1B	2.48	115.21	110.03
24	b	607	CLA	CMB-C2B-C3B	2.48	129.49	124.89
24	A	609	CLA	C4-C3-C5	2.48	119.59	115.29
31	t	103	LMT	C1B-O5B-C5B	2.48	118.39	113.72
38	h	101	HTG	O2-C2-C1	2.48	115.22	110.27
41	e	107	HEM	CMC-C2C-C3C	2.49	129.51	124.89
25	a	409	PHO	CMB-C2B-C1B	2.49	128.92	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	C3D-CAD-CBD	2.49	111.12	107.60
24	b	603	CLA	CED-O2D-CGD	2.49	121.81	115.97
41	E	113	HEM	CMC-C2C-C3C	2.50	129.52	124.89
31	A	617	LMT	C1B-O5B-C5B	2.50	118.42	113.72
24	a	410	CLA	C4-C3-C5	2.50	119.62	115.29
29	d	412	LMG	O3-C3-C4	2.50	115.81	110.36
28	a	424	SQD	O47-C45-C46	2.50	117.54	108.44
29	C	520	LMG	C9-O8-C28	2.51	124.67	117.13
31	J	103	LMT	O1'-C1'-C2'	2.51	112.32	108.23
38	O	303	HTG	C1'-S1-C1	2.51	104.00	100.28
40	H	103	DGD	O4E-C4E-C5E	2.51	115.61	109.28
24	a	410	CLA	CMC-C2C-C1C	2.51	128.83	125.02
40	D	408	DGD	C3G-O3G-C1D	2.52	118.92	113.76
38	a	418	HTG	O3-C3-C2	2.52	115.83	110.36
25	A	608	PHO	O2D-CGD-CBD	2.52	115.80	111.30
32	a	419	LHG	O7-C5-C4	2.52	117.61	108.44
24	a	410	CLA	C16-C15-C13	2.53	124.03	115.73
31	c	521	LMT	O1B-C1B-C2B	2.53	113.81	108.11
31	J	103	LMT	C1B-O1B-C4'	2.53	124.16	118.00
24	b	611	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	z	101	LMG	O1-C7-C8	2.53	117.02	110.99
31	A	617	LMT	O5B-C1B-C2B	2.54	115.19	110.30
38	b	623	HTG	O5-C5-C4	2.54	114.33	109.66
24	C	507	CLA	CMA-C3A-C4A	2.54	118.59	111.77
38	c	530	HTG	O5-C5-C4	2.54	114.34	109.66
31	J	103	LMT	C1'-C2'-C3'	2.55	114.72	109.98
24	b	612	CLA	CAC-C3C-C4C	2.55	128.43	124.83
24	B	605	CLA	CAC-C3C-C4C	2.55	128.43	124.83
24	D	404	CLA	CMB-C2B-C3B	2.56	129.64	124.89
28	b	633	SQD	C45-O47-C7	2.56	123.93	117.88
24	b	610	CLA	C1D-CHD-C4C	2.56	125.99	122.48
24	C	511	CLA	CAC-C3C-C4C	2.56	128.45	124.83
24	C	503	CLA	O2D-CGD-CBD	2.57	115.89	111.30
24	a	407	CLA	CMB-C2B-C3B	2.57	129.67	124.89
41	e	107	HEM	CBD-CAD-C3D	2.58	117.39	112.47
31	I	101	LMT	O1'-C1'-C2'	2.58	112.44	108.23
24	B	605	CLA	CAA-C2A-C1A	2.58	120.44	111.97
26	B	619	BCR	C37-C22-C23	2.58	122.22	118.10
38	B	623	HTG	O4-C4-C5	2.59	115.80	109.28
24	C	508	CLA	CMB-C2B-C3B	2.59	129.69	124.89
26	H	102	BCR	C28-C27-C26	2.59	118.25	113.78
29	B	634	LMG	C4-C3-C2	2.60	115.42	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	CMC-C2C-C1C	2.60	128.96	125.02
38	c	523	HTG	O5-C5-C4	2.60	114.45	109.66
41	v	202	HEM	CMA-C3A-C2A	2.60	129.85	124.94
24	B	612	CLA	O2D-CGD-CBD	2.60	115.95	111.30
24	B	604	CLA	C6-C5-C3	2.60	118.56	112.66
24	B	609	CLA	CMB-C2B-C3B	2.61	129.73	124.89
25	d	401	PHO	CAC-C3C-C4C	2.61	128.27	125.21
24	D	404	CLA	C2A-C3A-C4A	2.61	106.08	101.87
31	b	622	LMT	C3'-C4'-C5'	2.61	116.41	110.88
24	c	508	CLA	O2D-CGD-CBD	2.61	115.97	111.30
24	b	605	CLA	CMB-C2B-C3B	2.61	129.74	124.89
27	d	407	PL9	C20-C19-C21	2.61	119.82	115.29
24	a	410	CLA	CHB-C4A-NA	2.61	128.13	124.51
24	B	614	CLA	CAC-C3C-C4C	2.61	128.52	124.83
29	z	101	LMG	C3-C4-C5	2.62	114.83	110.22
31	t	103	LMT	O5B-C5B-C4B	2.63	114.50	109.66
24	c	513	CLA	O2A-CGA-CBA	2.63	119.55	111.90
24	c	503	CLA	CMB-C2B-C3B	2.63	129.77	124.89
26	h	103	BCR	C2-C1-C6	2.63	114.59	110.48
24	d	404	CLA	C3D-CAD-CBD	2.64	111.32	107.60
24	b	614	CLA	O2A-CGA-CBA	2.64	119.58	111.90
24	a	408	CLA	C4-C3-C5	2.64	119.87	115.29
31	I	101	LMT	C6B-C5B-C4B	2.64	119.19	113.00
24	b	604	CLA	CAC-C3C-C4C	2.64	128.56	124.83
27	d	407	PL9	C10-C9-C11	2.65	119.88	115.29
24	b	613	CLA	CMB-C2B-C3B	2.66	129.82	124.89
24	C	502	CLA	O2D-CGD-CBD	2.66	116.05	111.30
40	c	518	DGD	O6E-C5E-C6E	2.66	112.78	106.41
32	A	618	LHG	C6-O8-C23	2.66	125.14	117.13
29	B	634	LMG	C30-C29-C28	2.66	123.31	113.58
29	C	526	LMG	O6-C5-C4	2.67	114.57	109.66
30	c	525	GOL	O1-C1-C2	2.67	123.50	110.07
24	A	606	CLA	C4-C3-C5	2.67	119.91	115.29
29	a	414	LMG	C4-C3-C2	2.67	115.54	110.84
24	d	404	CLA	CHB-C4A-NA	2.67	128.20	124.51
24	C	512	CLA	CMC-C2C-C1C	2.67	129.07	125.02
24	a	410	CLA	C3D-CAD-CBD	2.68	111.38	107.60
24	C	509	CLA	O2A-CGA-CBA	2.68	119.69	111.90
24	B	609	CLA	C4-C3-C5	2.68	119.93	115.29
24	B	611	CLA	CMB-C2B-C3B	2.68	129.87	124.89
24	C	507	CLA	CMB-C2B-C3B	2.69	129.88	124.89
38	b	624	HTG	O4-C4-C3	2.69	116.21	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	CAC-C3C-C4C	2.69	128.62	124.83
24	C	503	CLA	CAA-C2A-C1A	2.69	120.80	111.97
25	a	409	PHO	CMC-C2C-C1C	2.69	129.24	125.04
24	C	512	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	k	101	BCR	C37-C22-C23	2.70	122.40	118.10
38	b	623	HTG	C2'-C1'-S1	2.70	121.27	112.45
24	c	513	CLA	CHB-C4A-NA	2.70	128.25	124.51
31	M	101	LMT	C1B-O1B-C4'	2.70	124.58	118.00
24	c	509	CLA	CHB-C4A-NA	2.70	128.25	124.51
27	D	407	PL9	C35-C34-C36	2.71	119.98	115.29
24	b	609	CLA	CMC-C2C-C1C	2.71	129.13	125.02
26	h	103	BCR	C36-C18-C19	2.71	122.42	118.10
24	c	511	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	A	610	BCR	C37-C22-C23	2.71	122.42	118.10
41	E	113	HEM	CAA-CBA-CGA	2.72	117.31	112.66
28	h	105	SQD	O5-C1-C2	2.72	115.54	110.30
29	A	613	LMG	C3-C4-C5	2.72	115.01	110.22
26	A	610	BCR	C2-C1-C6	2.72	114.73	110.48
24	B	615	CLA	CAC-C3C-C4C	2.72	128.67	124.83
38	H	101	HTG	C3-C4-C5	2.72	115.02	110.22
24	c	511	CLA	CMB-C2B-C3B	2.73	129.95	124.89
24	B	616	CLA	CAC-C3C-C4C	2.73	128.68	124.83
31	A	617	LMT	O3B-C3B-C4B	2.73	116.29	110.36
24	b	602	CLA	C3D-CAD-CBD	2.73	111.45	107.60
24	C	504	CLA	C1D-CHD-C4C	2.73	126.22	122.48
24	B	606	CLA	CAA-C2A-C1A	2.73	120.92	111.97
25	D	401	PHO	CAC-C3C-C4C	2.73	128.42	125.21
31	M	101	LMT	C1-O1'-C1'	2.73	118.56	113.87
24	B	614	CLA	CMB-C2B-C3B	2.73	129.97	124.89
38	C	521	HTG	O5-C5-C6	2.74	112.97	106.41
40	C	516	DGD	C1G-O1G-C1A	2.74	125.37	117.13
29	C	520	LMG	O1-C1-C2	2.75	112.72	108.23
28	A	622	SQD	O5-C5-C4	2.75	114.72	109.66
24	C	507	CLA	CAC-C3C-C4C	2.75	128.71	124.83
24	D	405	CLA	CMB-C2B-C3B	2.75	130.00	124.89
24	b	605	CLA	CAA-C2A-C1A	2.75	121.00	111.97
24	c	512	CLA	C1-O2A-CGA	2.76	123.38	116.77
31	a	401	LMT	O2'-C2'-C1'	2.76	115.80	110.03
40	h	104	DGD	O4E-C4E-C5E	2.76	116.24	109.28
24	D	405	CLA	CHB-C4A-NA	2.77	128.34	124.51
28	F	104	SQD	C46-O48-C23	2.77	125.47	117.13
38	C	532	HTG	O5-C5-C4	2.78	114.77	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	618	LHG	O7-C7-C8	2.78	117.33	111.55
26	k	101	BCR	C32-C1-C6	2.79	114.83	110.31
24	B	617	CLA	CMB-C2B-C3B	2.79	130.07	124.89
24	B	606	CLA	CHB-C4A-NA	2.79	128.37	124.51
38	B	624	HTG	C1-C2-C3	2.79	116.66	110.69
26	k	101	BCR	C29-C28-C27	2.79	117.99	111.34
24	b	603	CLA	CHB-C4A-NA	2.80	128.38	124.51
28	A	622	SQD	O6-C1-C2	2.80	112.80	108.23
24	c	512	CLA	CHB-C4A-NA	2.80	128.38	124.51
31	c	521	LMT	C1B-O1B-C4'	2.81	124.83	118.00
24	b	612	CLA	CMB-C2B-C3B	2.81	130.10	124.89
38	b	632	HTG	O5-C5-C6	2.81	113.13	106.41
24	c	508	CLA	C3D-CAD-CBD	2.81	111.57	107.60
24	b	609	CLA	C3D-CAD-CBD	2.81	111.57	107.60
31	t	103	LMT	C1'-C2'-C3'	2.82	115.22	109.98
40	h	104	DGD	O1G-C1A-C2A	2.82	120.10	111.90
26	B	620	BCR	C37-C22-C23	2.82	122.60	118.10
24	b	603	CLA	CMC-C2C-C1C	2.83	129.31	125.02
24	B	604	CLA	CMB-C2B-C3B	2.83	130.14	124.89
24	c	506	CLA	CHB-C4A-NA	2.83	128.42	124.51
24	b	615	CLA	CED-O2D-CGD	2.83	122.60	115.97
31	F	102	LMT	C1-O1'-C1'	2.83	118.73	113.87
24	A	609	CLA	CMC-C2C-C1C	2.83	129.32	125.02
24	c	509	CLA	CED-O2D-CGD	2.83	122.61	115.97
24	b	606	CLA	CAC-C3C-C4C	2.84	128.83	124.83
28	a	417	SQD	O7-S-C6	2.84	109.25	106.83
28	a	424	SQD	O6-C44-C45	2.84	117.75	110.99
24	B	615	CLA	O2A-CGA-CBA	2.84	120.18	111.90
28	h	105	SQD	O3-C3-C4	2.85	116.55	110.36
24	B	614	CLA	C3B-C4B-NB	2.85	112.89	109.21
24	c	502	CLA	O2D-CGD-CBD	2.85	116.39	111.30
26	c	514	BCR	C37-C22-C23	2.85	122.64	118.10
33	V	209	PG4	C7-O4-C6	2.85	125.66	113.30
30	C	528	GOL	O3-C3-C2	2.86	124.46	110.07
31	m	102	LMT	O5B-C5B-C4B	2.86	114.92	109.66
24	D	404	CLA	CMC-C2C-C1C	2.86	129.36	125.02
41	V	203	HEM	CMA-C3A-C2A	2.87	130.34	124.94
25	A	608	PHO	C2B-C1B-NB	2.87	114.07	109.82
38	b	632	HTG	C1-O5-C5	2.87	118.22	112.69
24	b	615	CLA	O2A-CGA-CBA	2.87	120.26	111.90
24	B	607	CLA	C4-C3-C5	2.89	120.30	115.29
38	C	530	HTG	O5-C5-C6	2.89	113.33	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	634	LMG	C9-O8-C28	2.89	125.84	117.13
26	C	515	BCR	C36-C18-C19	2.90	122.72	118.10
28	h	105	SQD	O48-C23-C24	2.90	120.33	111.90
32	l	101	LHG	O7-C7-C8	2.90	117.58	111.55
38	C	529	HTG	C1-O5-C5	2.90	118.28	112.69
24	c	502	CLA	C3D-CAD-CBD	2.91	111.70	107.60
24	C	513	CLA	O2A-CGA-CBA	2.91	120.36	111.90
38	B	624	HTG	O5-C1-C2	2.91	114.27	110.28
38	V	204	HTG	O2-C2-C1	2.92	116.08	110.27
32	d	410	LHG	O8-C23-C24	2.92	120.39	111.90
24	B	605	CLA	O2D-CGD-CBD	2.92	116.52	111.30
24	D	404	CLA	O2D-CGD-CBD	2.92	116.52	111.30
31	f	101	LMT	C1-O1'-C1'	2.92	118.88	113.87
25	d	401	PHO	C2B-C1B-NB	2.93	114.15	109.82
40	D	408	DGD	O6D-C5D-C6D	2.93	112.48	106.64
27	A	611	PL9	C35-C34-C36	2.93	120.37	115.29
31	j	103	LMT	C1B-O1B-C4'	2.93	125.14	118.00
40	D	408	DGD	O3G-C3G-C2G	2.93	117.97	110.99
24	b	608	CLA	CMC-C2C-C1C	2.94	129.47	125.02
24	B	611	CLA	CHB-C4A-NA	2.94	128.57	124.51
38	B	623	HTG	C1-C2-C3	2.94	116.98	110.69
24	B	611	CLA	C3D-CAD-CBD	2.95	111.76	107.60
28	h	105	SQD	O2-C2-C1	2.96	116.21	110.03
24	C	510	CLA	CMB-C2B-C3B	2.96	130.38	124.89
25	D	401	PHO	CMB-C2B-C1B	2.96	129.66	125.04
32	l	101	LHG	O8-C6-C5	2.96	116.11	108.66
31	m	101	LMT	O2'-C2'-C1'	2.97	116.24	110.03
38	V	204	HTG	O5-C1-S1	2.98	118.04	110.15
28	l	102	SQD	O9-S-C6	2.98	109.37	106.83
24	c	504	CLA	CHB-C4A-NA	2.98	128.63	124.51
26	t	102	BCR	C35-C13-C12	2.98	122.84	118.10
24	B	611	CLA	O2D-CGD-CBD	2.98	116.63	111.30
24	b	610	CLA	CMB-C2B-C3B	2.98	130.43	124.89
24	C	508	CLA	O2D-CGD-CBD	2.98	116.63	111.30
26	H	102	BCR	C36-C18-C19	2.99	122.86	118.10
24	b	607	CLA	O2D-CGD-CBD	2.99	116.64	111.30
28	h	105	SQD	O6-C1-C2	2.99	113.11	108.23
24	B	615	CLA	C1-O2A-CGA	2.99	123.95	116.77
26	H	102	BCR	C32-C1-C6	3.00	115.17	110.31
29	C	526	LMG	O3-C3-C4	3.00	116.88	110.36
26	c	515	BCR	C37-C22-C23	3.00	122.87	118.10
24	c	513	CLA	C3B-C4B-NB	3.00	113.09	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	C6-C5-C3	3.00	119.46	112.66
31	Y	101	LMT	C3B-C4B-C5B	3.00	115.51	110.22
24	C	512	CLA	C1-O2A-CGA	3.01	123.99	116.77
24	c	511	CLA	O2D-CGD-CBD	3.01	116.68	111.30
25	D	401	PHO	C4-C3-C5	3.01	120.52	115.29
28	x	101	SQD	O5-C5-C4	3.02	115.22	109.66
24	A	607	CLA	O2D-CGD-CBD	3.02	116.69	111.30
26	B	619	BCR	C39-C30-C25	3.02	115.21	110.31
24	A	607	CLA	CMB-C2B-C3B	3.02	130.50	124.89
38	a	418	HTG	C3-C4-C5	3.02	115.55	110.22
24	A	609	CLA	C3D-CAD-CBD	3.04	111.89	107.60
24	C	513	CLA	C3D-CAD-CBD	3.04	111.90	107.60
38	B	630	HTG	C4-C3-C2	3.05	116.21	110.84
29	B	634	LMG	C3-C4-C5	3.05	115.60	110.22
24	A	607	CLA	CMC-C2C-C1C	3.06	129.66	125.02
24	c	501	CLA	CMB-C2B-C3B	3.06	130.57	124.89
38	a	418	HTG	C1-O5-C5	3.06	118.59	112.69
24	b	613	CLA	CMC-C2C-C1C	3.06	129.66	125.02
26	C	525	BCR	C37-C22-C23	3.07	122.99	118.10
38	b	623	HTG	O5-C1-C2	3.07	114.49	110.28
24	b	609	CLA	O2D-CGD-CBD	3.08	116.80	111.30
24	b	608	CLA	C1D-CHD-C4C	3.08	126.69	122.48
31	M	101	LMT	O4'-C4B-C3B	3.09	117.08	110.36
24	B	611	CLA	CED-O2D-CGD	3.09	123.22	115.97
24	b	610	CLA	C6-C5-C3	3.09	119.67	112.66
24	b	614	CLA	CMC-C2C-C1C	3.10	129.72	125.02
29	B	634	LMG	C7-O1-C1	3.10	120.12	113.76
24	d	404	CLA	O2D-CGD-CBD	3.10	116.84	111.30
26	D	406	BCR	C29-C30-C25	3.10	115.33	110.48
24	B	611	CLA	CMC-C2C-C1C	3.11	129.73	125.02
27	a	412	PL9	C2-C1-C6	3.11	123.04	117.82
24	C	506	CLA	CAC-C3C-C4C	3.11	129.22	124.83
24	b	615	CLA	CAC-C3C-C4C	3.11	129.22	124.83
24	C	513	CLA	C3B-C4B-NB	3.12	113.24	109.21
24	b	608	CLA	CAC-C3C-C4C	3.12	129.23	124.83
31	M	101	LMT	O5'-C5'-C6'	3.12	113.89	106.41
26	C	515	BCR	C2-C3-C4	3.12	118.79	111.34
24	C	511	CLA	CMC-C2C-C1C	3.13	129.76	125.02
24	C	503	CLA	CAC-C3C-C4C	3.13	129.25	124.83
32	B	632	LHG	O7-C7-C8	3.13	118.06	111.55
26	H	102	BCR	C37-C22-C23	3.14	123.10	118.10
26	t	102	BCR	C37-C22-C23	3.14	123.10	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C4-C3-C5	3.14	120.75	115.29
29	j	101	LMG	O7-C10-C11	3.15	118.08	111.55
32	e	101	LHG	O8-C23-C24	3.15	121.06	111.90
29	C	519	LMG	O8-C9-C8	3.15	116.57	108.66
31	J	103	LMT	C3B-C4B-C5B	3.15	115.77	110.22
31	c	521	LMT	O3'-C3'-C4'	3.16	117.05	109.87
32	B	632	LHG	O4-P-O5	3.16	128.63	112.28
24	b	616	CLA	CHB-C4A-NA	3.16	128.88	124.51
26	d	406	BCR	C32-C1-C6	3.16	115.44	110.31
38	b	624	HTG	O5-C1-C2	3.18	114.63	110.28
38	C	531	HTG	C1'-S1-C1	3.18	105.00	100.28
24	D	404	CLA	CHB-C4A-NA	3.18	128.92	124.51
24	B	610	CLA	CAC-C3C-C4C	3.19	129.32	124.83
38	b	632	HTG	C3-C4-C5	3.19	115.84	110.22
40	D	408	DGD	O1G-C1A-C2A	3.19	121.19	111.90
24	b	603	CLA	CAC-C3C-C4C	3.20	129.34	124.83
31	F	102	LMT	C1'-O5'-C5'	3.20	119.74	113.72
24	c	511	CLA	CAA-C2A-C1A	3.20	122.47	111.97
40	C	518	DGD	O1G-C1A-C2A	3.20	121.22	111.90
24	b	607	CLA	C3B-C4B-NB	3.21	113.36	109.21
38	C	529	HTG	O5-C5-C6	3.21	114.10	106.41
38	C	530	HTG	C1'-S1-C1	3.22	105.06	100.28
38	B	630	HTG	C1'-S1-C1	3.22	105.06	100.28
40	d	408	DGD	O1G-C1A-C2A	3.22	121.28	111.90
29	A	613	LMG	O1-C1-C2	3.23	113.50	108.23
31	A	617	LMT	C1'-O5'-C5'	3.23	119.79	113.72
29	C	520	LMG	C4-C3-C2	3.24	116.54	110.84
26	t	102	BCR	C36-C18-C19	3.24	123.26	118.10
24	C	502	CLA	C3D-CAD-CBD	3.25	112.18	107.60
24	b	604	CLA	C4-C3-C5	3.26	120.94	115.29
24	B	609	CLA	CMC-C2C-C1C	3.26	129.97	125.02
24	c	512	CLA	CMC-C2C-C1C	3.26	129.97	125.02
24	C	506	CLA	C3B-C4B-NB	3.27	113.44	109.21
29	c	520	LMG	O8-C28-C29	3.28	121.43	111.90
24	B	612	CLA	CMB-C2B-C3B	3.29	130.99	124.89
31	M	101	LMT	C1B-C2B-C3B	3.29	116.09	109.98
28	x	101	SQD	C3-C4-C5	3.29	116.01	110.22
24	c	502	CLA	CAC-C3C-C4C	3.29	129.47	124.83
31	F	102	LMT	O5'-C5'-C6'	3.29	114.29	106.41
29	B	634	LMG	O8-C28-C29	3.29	121.47	111.90
24	b	616	CLA	O2D-CGD-CBD	3.29	117.18	111.30
29	c	520	LMG	O7-C10-C11	3.29	118.39	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	F	102	LMT	C1B-O5B-C5B	3.30	119.92	113.72
24	C	503	CLA	CMB-C2B-C3B	3.30	131.01	124.89
28	A	616	SQD	C44-O6-C1	3.30	120.53	113.76
29	d	412	LMG	O7-C10-C11	3.30	118.41	111.55
24	c	509	CLA	CMC-C2C-C1C	3.31	130.04	125.02
28	b	633	SQD	O47-C45-C46	3.31	120.47	108.44
24	B	602	CLA	CAC-C3C-C4C	3.31	129.50	124.83
31	M	102	LMT	O1'-C1'-C2'	3.31	113.64	108.23
24	A	606	CLA	CMB-C2B-C3B	3.32	131.04	124.89
25	A	608	PHO	C2D-C1D-ND	3.32	114.73	109.82
31	B	622	LMT	C3B-C4B-C5B	3.32	116.06	110.22
24	b	602	CLA	CHB-C4A-NA	3.33	129.11	124.51
24	B	602	CLA	C6-C5-C3	3.33	120.21	112.66
24	D	405	CLA	CAC-C3C-C4C	3.33	129.53	124.83
24	c	506	CLA	CED-O2D-CGD	3.34	123.80	115.97
24	c	505	CLA	CMB-C2B-C3B	3.34	131.09	124.89
28	a	424	SQD	O5-C5-C4	3.34	115.81	109.66
26	d	406	BCR	C38-C26-C27	3.35	119.80	113.45
24	c	505	CLA	CMC-C2C-C1C	3.35	130.10	125.02
31	m	102	LMT	C1B-C2B-C3B	3.35	116.21	109.98
38	c	531	HTG	C1-O5-C5	3.36	119.16	112.69
29	c	520	LMG	O1-C1-C2	3.36	113.72	108.23
31	a	401	LMT	O1'-C1'-C2'	3.36	113.72	108.23
40	h	104	DGD	O2G-C1B-C2B	3.37	118.54	111.55
24	C	501	CLA	CAC-C3C-C4C	3.37	129.58	124.83
24	d	403	CLA	C4-C3-C5	3.37	121.14	115.29
24	b	607	CLA	CAC-C3C-C4C	3.37	129.58	124.83
29	C	520	LMG	O7-C10-C11	3.37	118.56	111.55
24	B	609	CLA	O2D-CGD-CBD	3.38	117.33	111.30
32	D	409	LHG	C6-O8-C23	3.38	127.30	117.13
31	J	103	LMT	O3'-C3'-C4'	3.39	117.58	109.87
38	C	532	HTG	C3-C4-C5	3.39	116.19	110.22
32	d	409	LHG	C6-O8-C23	3.40	127.35	117.13
24	C	510	CLA	CED-O2D-CGD	3.40	123.95	115.97
24	B	608	CLA	CMB-C2B-C3B	3.41	131.21	124.89
24	B	617	CLA	CED-O2D-CGD	3.41	123.96	115.97
31	u	203	LMT	O1B-C1B-C2B	3.41	115.80	108.11
31	t	103	LMT	C4B-C3B-C2B	3.42	116.87	110.84
31	j	103	LMT	O1B-C1B-C2B	3.42	115.82	108.11
31	b	622	LMT	O5'-C5'-C4'	3.42	116.76	109.75
28	F	104	SQD	O48-C23-C24	3.43	121.88	111.90
24	A	609	CLA	O2D-CGD-CBD	3.43	117.42	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	652	P6G	O4-C3-C2	3.43	126.00	110.15
24	B	614	CLA	O2A-CGA-CBA	3.44	121.90	111.90
31	J	103	LMT	O5B-C5B-C4B	3.44	115.99	109.66
24	b	611	CLA	C3B-C4B-NB	3.45	113.67	109.21
32	A	618	LHG	O8-C6-C5	3.45	117.33	108.66
31	I	101	LMT	O3'-C3'-C4'	3.45	117.73	109.87
24	c	504	CLA	CMB-C2B-C3B	3.45	131.30	124.89
29	C	520	LMG	O8-C28-C29	3.45	121.95	111.90
28	a	417	SQD	O47-C7-C8	3.46	118.74	111.55
31	Y	101	LMT	O1B-C1B-C2B	3.46	115.92	108.11
24	d	405	CLA	CMC-C2C-C1C	3.47	130.29	125.02
24	B	617	CLA	O2A-CGA-CBA	3.48	122.03	111.90
24	b	611	CLA	O2D-CGD-CBD	3.49	117.53	111.30
24	B	606	CLA	CMC-C2C-C1C	3.49	130.31	125.02
31	f	101	LMT	O4'-C4B-C5B	3.49	118.09	109.28
24	b	610	CLA	CAC-C3C-C4C	3.50	129.76	124.83
25	D	401	PHO	C2C-C1C-NC	3.50	115.00	109.82
40	d	408	DGD	C1E-O6E-C5E	3.50	120.31	113.72
24	C	505	CLA	O2D-CGD-CBD	3.51	117.57	111.30
24	c	510	CLA	CAC-C3C-C4C	3.51	129.78	124.83
24	d	405	CLA	C4-C3-C5	3.51	121.38	115.29
25	D	401	PHO	CED-O2D-CGD	3.51	124.21	115.97
26	h	103	BCR	C37-C22-C23	3.52	123.71	118.10
24	B	611	CLA	C3B-C4B-NB	3.52	113.77	109.21
24	C	502	CLA	CAC-C3C-C4C	3.53	129.81	124.83
38	a	418	HTG	O2-C2-C3	3.54	118.05	110.36
24	b	602	CLA	CED-O2D-CGD	3.54	124.28	115.97
24	B	606	CLA	CAC-C3C-C4C	3.54	129.83	124.83
24	a	408	CLA	O2D-CGD-CBD	3.55	117.64	111.30
24	a	408	CLA	CMC-C2C-C1C	3.55	130.40	125.02
24	C	504	CLA	O2D-CGD-CBD	3.56	117.66	111.30
24	b	602	CLA	CAC-C3C-C4C	3.57	129.86	124.83
31	f	101	LMT	C1B-O5B-C5B	3.57	120.44	113.72
24	d	404	CLA	CMC-C2C-C1C	3.57	130.44	125.02
24	B	615	CLA	CED-O2D-CGD	3.57	124.34	115.97
28	h	105	SQD	O47-C7-C8	3.58	118.98	111.55
38	b	631	HTG	C4-C3-C2	3.60	117.18	110.84
24	b	616	CLA	C3B-C4B-NB	3.60	113.86	109.21
32	A	618	LHG	O8-C23-C24	3.60	122.37	111.90
24	c	512	CLA	O2A-CGA-CBA	3.61	122.39	111.90
40	d	408	DGD	C2G-O2G-C1B	3.61	126.40	117.88
24	b	602	CLA	C1-O2A-CGA	3.62	125.45	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	403	CLA	CAC-C3C-C4C	3.62	129.94	124.83
24	B	613	CLA	CAC-C3C-C4C	3.62	129.94	124.83
24	C	507	CLA	O2D-CGD-CBD	3.63	117.78	111.30
24	d	404	CLA	C4-C3-C5	3.63	121.59	115.29
30	C	523	GOL	O2-C2-C1	3.63	125.99	108.84
24	C	513	CLA	C4-C3-C5	3.63	121.59	115.29
31	M	101	LMT	O1'-C1'-C2'	3.64	114.17	108.23
24	a	408	CLA	CAC-C3C-C4C	3.64	129.97	124.83
24	B	615	CLA	O2D-CGD-CBD	3.64	117.81	111.30
28	A	612	SQD	O2-C2-C1	3.64	117.65	110.03
31	u	203	LMT	C3B-C4B-C5B	3.65	116.64	110.22
24	b	605	CLA	O2D-CGD-CBD	3.65	117.83	111.30
28	a	424	SQD	C46-O48-C23	3.66	128.15	117.13
24	c	510	CLA	C3B-C4B-NB	3.67	113.95	109.21
24	a	410	CLA	CAC-C3C-C4C	3.67	130.01	124.83
28	A	616	SQD	O48-C23-C24	3.67	122.59	111.90
24	B	603	CLA	CMC-C2C-C1C	3.68	130.60	125.02
24	B	610	CLA	CMB-C2B-C3B	3.69	131.73	124.89
24	B	602	CLA	CHB-C4A-NA	3.69	129.61	124.51
26	D	406	BCR	C40-C30-C39	3.69	119.81	108.50
38	o	301	HTG	C1'-S1-C1	3.69	105.76	100.28
24	c	507	CLA	CMC-C2C-C1C	3.69	130.62	125.02
24	c	506	CLA	CMC-C2C-C1C	3.70	130.62	125.02
24	C	510	CLA	C3B-C4B-NB	3.70	113.99	109.21
25	A	608	PHO	CAC-C3C-C4C	3.70	129.56	125.21
24	C	504	CLA	CMC-C2C-C1C	3.70	130.63	125.02
38	b	632	HTG	C1'-S1-C1	3.71	105.78	100.28
31	F	102	LMT	O4'-C4B-C5B	3.71	118.63	109.28
28	A	616	SQD	O9-S-C6	3.71	110.00	106.83
24	c	504	CLA	O2D-CGD-CBD	3.72	117.94	111.30
28	l	102	SQD	O48-C23-C24	3.72	122.72	111.90
24	C	512	CLA	O2D-CGD-CBD	3.72	117.95	111.30
38	c	522	HTG	C1'-S1-C1	3.74	105.82	100.28
24	B	613	CLA	C3B-C4B-NB	3.75	114.05	109.21
29	c	520	LMG	C4-C3-C2	3.75	117.45	110.84
25	a	409	PHO	O2D-CGD-CBD	3.75	118.01	111.30
24	B	615	CLA	C3B-C4B-NB	3.75	114.06	109.21
31	Y	101	LMT	O1B-C4'-C3'	3.76	116.24	107.19
24	c	513	CLA	CMB-C2B-C3B	3.76	131.87	124.89
24	D	405	CLA	O2D-CGD-CBD	3.77	118.03	111.30
24	A	607	CLA	C3B-C4B-NB	3.77	114.09	109.21
28	h	105	SQD	O48-C46-C45	3.78	118.16	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	CMC-C2C-C1C	3.78	130.76	125.02
24	C	505	CLA	CMB-C2B-C3B	3.79	131.92	124.89
24	b	604	CLA	O2D-CGD-CBD	3.79	118.07	111.30
24	b	603	CLA	CMB-C2B-C3B	3.80	131.94	124.89
28	F	104	SQD	C3-C4-C5	3.80	116.91	110.22
24	B	612	CLA	CAC-C3C-C4C	3.80	130.19	124.83
26	D	406	BCR	C32-C1-C6	3.80	116.48	110.31
26	D	406	BCR	C37-C22-C23	3.82	124.18	118.10
24	c	511	CLA	C3B-C4B-NB	3.82	114.15	109.21
24	c	507	CLA	CAC-C3C-C4C	3.84	130.24	124.83
24	b	617	CLA	CMB-C2B-C3B	3.84	132.01	124.89
29	z	101	LMG	O7-C10-C11	3.86	119.56	111.55
24	B	606	CLA	C3B-C4B-NB	3.86	114.20	109.21
24	b	606	CLA	O2D-CGD-CBD	3.86	118.19	111.30
24	C	507	CLA	C3B-C4B-NB	3.86	114.20	109.21
40	D	408	DGD	O5D-C6D-C5D	3.88	115.44	108.94
24	a	407	CLA	CMC-C2C-C1C	3.89	130.91	125.02
25	d	401	PHO	C4-C3-C5	3.90	122.05	115.29
24	B	602	CLA	O2A-CGA-CBA	3.90	123.26	111.90
24	c	503	CLA	CMC-C2C-C1C	3.91	130.95	125.02
41	e	107	HEM	CAD-CBD-CGD	3.91	119.35	112.66
31	u	203	LMT	C1B-O5B-C5B	3.92	121.10	113.72
28	A	622	SQD	O48-C23-C24	3.93	123.33	111.90
31	u	203	LMT	O1'-C1'-C2'	3.93	114.65	108.23
25	a	409	PHO	C3C-C4C-NC	3.94	116.62	110.19
38	c	530	HTG	C1'-S1-C1	3.94	106.12	100.28
24	b	611	CLA	CED-O2D-CGD	3.94	125.20	115.97
24	C	507	CLA	CMC-C2C-C1C	3.94	130.99	125.02
40	D	408	DGD	C2G-O2G-C1B	3.94	127.19	117.88
28	a	413	SQD	O47-C7-C8	3.94	119.74	111.55
28	a	424	SQD	O48-C23-C24	3.95	123.39	111.90
24	b	602	CLA	CMC-C2C-C1C	3.95	131.01	125.02
24	b	603	CLA	O2D-CGD-CBD	3.96	118.37	111.30
24	A	607	CLA	C4-C3-C5	3.96	122.16	115.29
24	C	504	CLA	C3C-C4C-NC	3.96	114.22	110.21
24	C	505	CLA	CMC-C2C-C1C	3.97	131.04	125.02
40	c	516	DGD	O2G-C1B-C2B	3.97	119.80	111.55
31	J	103	LMT	C1B-O5B-C5B	3.99	121.24	113.72
27	d	407	PL9	C40-C39-C41	4.00	122.22	115.29
24	B	602	CLA	C3B-C4B-NB	4.00	114.38	109.21
24	b	617	CLA	C3B-C4B-NB	4.01	114.39	109.21
24	b	615	CLA	CMC-C2C-C1C	4.01	131.10	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	604	CLA	CMC-C2C-C1C	4.01	131.11	125.02
24	B	614	CLA	C1D-CHD-C4C	4.01	127.97	122.48
31	j	103	LMT	C3B-C4B-C5B	4.02	117.30	110.22
24	C	509	CLA	CMC-C2C-C1C	4.02	131.11	125.02
24	c	507	CLA	O2D-CGD-CBD	4.03	118.49	111.30
24	C	502	CLA	C3C-C4C-NC	4.03	114.29	110.21
28	l	102	SQD	O8-S-C6	4.03	110.93	106.01
24	B	613	CLA	O2D-CGD-CBD	4.04	118.53	111.30
31	u	203	LMT	O5B-C5B-C6B	4.06	116.12	106.41
24	b	606	CLA	C3B-C4B-NB	4.06	114.45	109.21
24	b	612	CLA	O2D-CGD-CBD	4.07	118.56	111.30
25	D	401	PHO	C2B-C1B-NB	4.07	115.84	109.82
31	f	101	LMT	O5'-C5'-C6'	4.07	116.15	106.41
24	C	513	CLA	CAC-C3C-C4C	4.08	130.58	124.83
26	K	101	BCR	C37-C22-C23	4.08	124.59	118.10
24	b	611	CLA	CMC-C2C-C1C	4.08	131.21	125.02
27	A	611	PL9	C2-C1-C6	4.09	124.69	117.82
28	a	424	SQD	O6-C1-C2	4.10	114.93	108.23
25	d	401	PHO	O2D-CGD-CBD	4.12	118.66	111.30
27	a	412	PL9	C53-C6-C1	4.12	123.59	114.84
24	B	608	CLA	CMC-C2C-C1C	4.13	131.28	125.02
31	A	617	LMT	C1-O1'-C1'	4.13	120.96	113.87
24	A	609	CLA	CED-O2D-CGD	4.13	125.66	115.97
24	c	509	CLA	C3B-C4B-NB	4.14	114.57	109.21
24	C	510	CLA	CAC-C3C-C4C	4.14	130.67	124.83
24	C	501	CLA	CMC-C2C-C1C	4.15	131.31	125.02
29	c	519	LMG	O7-C10-C11	4.15	120.17	111.55
24	B	603	CLA	O2D-CGD-CBD	4.15	118.72	111.30
24	B	617	CLA	CAC-C3C-C4C	4.16	130.70	124.83
24	B	617	CLA	C3B-C4B-NB	4.16	114.59	109.21
24	A	609	CLA	C3B-C4B-NB	4.17	114.60	109.21
31	b	622	LMT	O1'-C1'-C2'	4.17	115.03	108.23
31	C	533	LMT	O1B-C4'-C3'	4.17	117.22	107.19
24	c	505	CLA	C3B-C4B-NB	4.17	114.60	109.21
24	a	407	CLA	C3B-C4B-NB	4.17	114.61	109.21
28	A	622	SQD	C45-O47-C7	4.17	127.74	117.88
24	B	610	CLA	CMC-C2C-C1C	4.18	131.36	125.02
24	d	403	CLA	C3B-C4B-NB	4.19	114.62	109.21
24	b	605	CLA	CMC-C2C-C1C	4.21	131.40	125.02
24	b	603	CLA	C3B-C4B-NB	4.21	114.66	109.21
38	h	101	HTG	O5-C1-C2	4.23	116.08	110.28
24	C	505	CLA	C3B-C4B-NB	4.24	114.69	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	CMB-C2B-C3B	4.24	132.76	124.89
28	b	633	SQD	O47-C7-C8	4.24	120.36	111.55
28	b	633	SQD	O48-C23-C24	4.25	124.27	111.90
24	A	606	CLA	CAC-C3C-C4C	4.26	130.83	124.83
24	b	615	CLA	C3B-C4B-NB	4.27	114.72	109.21
24	B	602	CLA	C3D-CAD-CBD	4.27	113.63	107.60
24	C	505	CLA	CAC-C3C-C4C	4.28	130.87	124.83
24	C	506	CLA	O2D-CGD-CBD	4.29	118.96	111.30
24	B	611	CLA	CAC-C3C-C4C	4.29	130.88	124.83
28	x	101	SQD	O48-C23-C24	4.29	124.38	111.90
28	A	616	SQD	O6-C1-C2	4.29	115.23	108.23
31	u	203	LMT	O5B-C1B-C2B	4.33	118.65	110.30
24	A	606	CLA	C3B-C4B-NB	4.33	114.81	109.21
24	c	503	CLA	C3B-C4B-NB	4.34	114.82	109.21
26	d	406	BCR	C40-C30-C39	4.35	121.82	108.50
26	b	619	BCR	C37-C22-C23	4.35	125.02	118.10
24	B	616	CLA	CMC-C2C-C1C	4.37	131.65	125.02
38	H	101	HTG	C1-O5-C5	4.37	121.11	112.69
28	l	102	SQD	O47-C7-C8	4.38	120.64	111.55
24	C	512	CLA	CAC-C3C-C4C	4.39	131.02	124.83
31	B	622	LMT	O1'-C1'-C2'	4.40	115.41	108.23
29	B	634	LMG	O7-C10-C11	4.40	120.68	111.55
24	b	605	CLA	C3B-C4B-NB	4.40	114.89	109.21
28	x	101	SQD	C1-O5-C5	4.41	122.01	113.72
24	b	616	CLA	CMB-C2B-C3B	4.41	133.08	124.89
24	a	407	CLA	CAC-C3C-C4C	4.42	131.06	124.83
24	c	502	CLA	C3B-C4B-NB	4.43	114.94	109.21
32	D	409	LHG	O8-C23-C24	4.43	124.80	111.90
40	d	408	DGD	C3G-O3G-C1D	4.44	122.86	113.76
32	d	409	LHG	O8-C23-C24	4.44	124.82	111.90
24	C	513	CLA	O2D-CGD-CBD	4.45	119.25	111.30
24	c	502	CLA	CMC-C2C-C1C	4.46	131.78	125.02
27	A	611	PL9	C53-C6-C1	4.46	124.31	114.84
24	C	504	CLA	C3B-C4B-NB	4.46	114.98	109.21
24	d	405	CLA	CAC-C3C-C4C	4.47	131.13	124.83
38	B	631	HTG	C1'-S1-C1	4.50	106.95	100.28
28	l	102	SQD	O2-C2-C1	4.52	119.47	110.03
29	C	519	LMG	O7-C10-C11	4.53	120.95	111.55
28	x	101	SQD	O47-C7-C8	4.53	120.95	111.55
31	j	103	LMT	C1-O1'-C1'	4.53	121.64	113.87
40	C	516	DGD	O2G-C1B-C2B	4.54	120.97	111.55
24	c	504	CLA	CMC-C2C-C1C	4.55	131.91	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	C3B-C4B-NB	4.55	115.10	109.21
40	C	517	DGD	O2G-C1B-C2B	4.55	121.01	111.55
24	C	510	CLA	CMC-C2C-C1C	4.56	131.93	125.02
24	C	506	CLA	CMC-C2C-C1C	4.57	131.95	125.02
28	l	102	SQD	O48-C46-C45	4.57	120.14	108.66
28	b	633	SQD	C4-C3-C2	4.58	118.91	110.84
24	b	608	CLA	C3B-C4B-NB	4.58	115.13	109.21
24	d	405	CLA	O2D-CGD-CBD	4.58	119.49	111.30
24	B	609	CLA	C3B-C4B-NB	4.59	115.15	109.21
28	a	417	SQD	O48-C23-C24	4.60	125.28	111.90
38	C	522	HTG	C1-O5-C5	4.61	121.56	112.69
25	a	409	PHO	C2C-C1C-NC	4.61	116.64	109.82
24	b	611	CLA	CAC-C3C-C4C	4.62	131.34	124.83
24	D	405	CLA	C3B-C4B-NB	4.62	115.19	109.21
24	b	610	CLA	C3B-C4B-NB	4.63	115.19	109.21
24	b	613	CLA	CAC-C3C-C4C	4.63	131.36	124.83
24	B	604	CLA	C3B-C4B-NB	4.64	115.22	109.21
24	c	501	CLA	O2D-CGD-CBD	4.65	119.60	111.30
27	D	407	PL9	C40-C39-C41	4.67	123.39	115.29
28	A	622	SQD	C44-O6-C1	4.69	123.37	113.76
24	b	617	CLA	CAC-C3C-C4C	4.69	131.44	124.83
24	b	614	CLA	C3B-C4B-NB	4.69	115.27	109.21
24	b	606	CLA	CMC-C2C-C1C	4.71	132.16	125.02
38	C	532	HTG	C1-O5-C5	4.71	121.76	112.69
24	b	605	CLA	CAC-C3C-C4C	4.71	131.48	124.83
24	C	502	CLA	CMC-C2C-C1C	4.72	132.17	125.02
25	D	401	PHO	C3C-C4C-NC	4.74	117.94	110.19
28	h	105	SQD	O9-S-C6	4.77	110.91	106.83
24	c	507	CLA	C3B-C4B-NB	4.78	115.39	109.21
28	A	612	SQD	O6-C1-C2	4.78	116.04	108.23
24	b	613	CLA	C3B-C4B-NB	4.80	115.41	109.21
32	E	101	LHG	O7-C7-C8	4.80	121.53	111.55
24	C	511	CLA	C3B-C4B-NB	4.80	115.42	109.21
24	C	509	CLA	CAC-C3C-C4C	4.81	131.61	124.83
24	b	609	CLA	C3B-C4B-NB	4.81	115.43	109.21
24	c	501	CLA	CMC-C2C-C1C	4.81	132.31	125.02
28	F	104	SQD	O7-S-C6	4.81	110.94	106.83
24	c	509	CLA	CAC-C3C-C4C	4.81	131.62	124.83
28	a	424	SQD	O8-S-C6	4.82	111.89	106.01
24	b	610	CLA	O2D-CGD-CBD	4.82	119.92	111.30
24	B	605	CLA	C3B-C4B-NB	4.83	115.46	109.21
24	B	607	CLA	CMC-C2C-C1C	4.84	132.36	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	CAC-C3C-C4C	4.85	131.67	124.83
24	B	603	CLA	C3B-C4B-NB	4.85	115.48	109.21
28	A	616	SQD	O47-C7-C8	4.87	121.66	111.55
27	a	412	PL9	C3-C4-C5	4.88	125.18	118.63
24	c	510	CLA	O2D-CGD-CBD	4.88	120.02	111.30
24	d	405	CLA	C3B-C4B-NB	4.88	115.53	109.21
24	b	612	CLA	C3B-C4B-NB	4.89	115.53	109.21
24	a	407	CLA	C3C-C4C-NC	4.91	115.19	110.21
31	A	617	LMT	O2'-C2'-C1'	4.91	120.30	110.03
29	a	414	LMG	O7-C10-C11	4.91	121.76	111.55
38	c	523	HTG	C1'-S1-C1	4.95	107.62	100.28
24	C	508	CLA	C3B-C4B-NB	4.95	115.61	109.21
24	B	610	CLA	C3B-C4B-NB	4.96	115.62	109.21
24	C	509	CLA	C3B-C4B-NB	4.96	115.62	109.21
24	B	608	CLA	C3B-C4B-NB	4.98	115.64	109.21
24	b	615	CLA	O2D-CGD-CBD	4.98	120.20	111.30
24	c	512	CLA	O2D-CGD-CBD	5.00	120.24	111.30
24	b	616	CLA	C3C-C4C-NC	5.01	115.28	110.21
24	C	501	CLA	C3B-C4B-NB	5.02	115.70	109.21
28	a	424	SQD	C44-O6-C1	5.04	124.08	113.76
24	b	616	CLA	CMC-C2C-C1C	5.05	132.68	125.02
30	C	528	GOL	C3-C2-C1	5.11	131.81	111.52
31	a	401	LMT	C1'-O5'-C5'	5.11	123.34	113.72
25	d	401	PHO	CMD-C2D-C1D	5.11	133.00	125.04
25	A	608	PHO	C2C-C1C-NC	5.11	117.39	109.82
24	c	512	CLA	C3B-C4B-NB	5.12	115.83	109.21
24	c	508	CLA	C3B-C4B-NB	5.13	115.85	109.21
40	c	517	DGD	O2G-C1B-C2B	5.14	122.21	111.55
25	a	409	PHO	CMD-C2D-C1D	5.14	133.04	125.04
32	e	101	LHG	O7-C7-C8	5.14	122.22	111.55
24	C	503	CLA	CMC-C2C-C1C	5.16	132.85	125.02
24	D	404	CLA	C3B-C4B-NB	5.16	115.89	109.21
24	c	504	CLA	C3C-C4C-NC	5.17	115.45	110.21
28	F	104	SQD	O3-C3-C2	5.18	121.62	110.36
24	b	612	CLA	CMC-C2C-C1C	5.20	132.90	125.02
24	C	503	CLA	C3B-C4B-NB	5.20	115.94	109.21
24	B	617	CLA	O2D-CGD-CBD	5.21	120.61	111.30
25	d	401	PHO	C3C-C4C-NC	5.24	118.75	110.19
24	b	604	CLA	C3B-C4B-NB	5.24	115.99	109.21
25	d	401	PHO	C2C-C1C-NC	5.25	117.60	109.82
24	c	503	CLA	C3C-C4C-NC	5.26	115.54	110.21
28	A	612	SQD	O8-S-C6	5.26	112.44	106.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	609	CLA	C3C-C4C-NC	5.28	115.56	110.21
24	c	501	CLA	C3C-C4C-NC	5.30	115.58	110.21
24	c	502	CLA	C3C-C4C-NC	5.30	115.58	110.21
24	B	612	CLA	CMC-C2C-C1C	5.30	133.06	125.02
24	b	617	CLA	O2A-CGA-CBA	5.31	127.36	111.90
24	b	615	CLA	C3C-C4C-NC	5.34	115.62	110.21
29	c	519	LMG	O8-C28-C29	5.34	127.44	111.90
24	a	410	CLA	C3B-C4B-NB	5.35	116.12	109.21
24	C	501	CLA	C3C-C4C-NC	5.35	115.63	110.21
24	B	607	CLA	O2D-CGD-CBD	5.36	120.87	111.30
25	A	608	PHO	CMD-C2D-C1D	5.38	133.43	125.04
40	D	408	DGD	O3G-C1D-C2D	5.38	117.02	108.23
24	B	615	CLA	C3C-C4C-NC	5.39	115.67	110.21
29	b	621	LMG	O7-C10-C11	5.41	122.78	111.55
24	B	613	CLA	C3C-C4C-NC	5.41	115.69	110.21
24	C	511	CLA	O2D-CGD-CBD	5.43	121.00	111.30
25	A	608	PHO	C3C-C4C-NC	5.43	119.06	110.19
24	A	607	CLA	CAC-C3C-C4C	5.45	132.51	124.83
24	B	604	CLA	O2D-CGD-CBD	5.45	121.05	111.30
24	b	607	CLA	C3C-C4C-NC	5.47	115.75	110.21
28	A	612	SQD	O47-C7-C8	5.47	122.91	111.55
24	C	512	CLA	C3B-C4B-NB	5.49	116.31	109.21
24	c	511	CLA	C3C-C4C-NC	5.52	115.80	110.21
24	a	408	CLA	C3B-C4B-NB	5.52	116.35	109.21
24	B	604	CLA	C3C-C4C-NC	5.54	115.83	110.21
28	F	104	SQD	O8-S-C6	5.55	112.78	106.01
24	B	604	CLA	CMC-C2C-C1C	5.56	133.44	125.02
24	C	511	CLA	C3C-C4C-NC	5.56	115.85	110.21
31	m	102	LMT	O1'-C1'-C2'	5.57	117.32	108.23
24	c	511	CLA	CMC-C2C-C1C	5.58	133.47	125.02
24	B	607	CLA	C3B-C4B-NB	5.58	116.43	109.21
28	b	633	SQD	O6-C1-C2	5.61	117.39	108.23
24	B	608	CLA	C3C-C4C-NC	5.61	115.90	110.21
24	D	403	CLA	C3B-C4B-NB	5.62	116.47	109.21
24	b	617	CLA	O2D-CGD-CBD	5.64	121.38	111.30
24	c	506	CLA	C3B-C4B-NB	5.65	116.52	109.21
24	C	502	CLA	C3B-C4B-NB	5.67	116.54	109.21
24	c	505	CLA	CAC-C3C-C4C	5.69	132.85	124.83
26	t	102	BCR	C31-C1-C6	5.69	119.54	110.31
24	B	616	CLA	C3B-C4B-NB	5.74	116.63	109.21
24	b	604	CLA	C3C-C4C-NC	5.74	116.03	110.21
29	b	621	LMG	O8-C28-C29	5.74	128.62	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	419	LHG	O7-C7-C8	5.76	123.52	111.55
29	B	621	LMG	O8-C28-C29	5.77	128.68	111.90
24	C	509	CLA	C3C-C4C-NC	5.77	116.06	110.21
31	I	101	LMT	O1B-C4'-C3'	5.77	121.08	107.19
24	d	403	CLA	C3C-C4C-NC	5.78	116.06	110.21
29	C	526	LMG	O7-C10-C11	5.78	123.56	111.55
24	b	612	CLA	C3C-C4C-NC	5.80	116.08	110.21
24	B	607	CLA	C3C-C4C-NC	5.80	116.09	110.21
24	D	403	CLA	C3C-C4C-NC	5.83	116.12	110.21
24	c	512	CLA	C3C-C4C-NC	5.87	116.16	110.21
24	c	513	CLA	CMC-C2C-C1C	5.88	133.93	125.02
24	B	613	CLA	C2C-C1C-NC	5.93	114.30	110.22
24	c	501	CLA	C3B-C4B-NB	5.93	116.88	109.21
24	d	404	CLA	C3C-C4C-NC	5.95	116.24	110.21
25	D	401	PHO	CMD-C2D-C1D	5.98	134.35	125.04
24	B	602	CLA	CMC-C2C-C1C	5.99	134.10	125.02
24	b	608	CLA	C3C-C4C-NC	6.01	116.30	110.21
24	d	405	CLA	C3C-C4C-NC	6.07	116.36	110.21
24	C	512	CLA	C3C-C4C-NC	6.08	116.37	110.21
24	A	606	CLA	C3C-C4C-NC	6.09	116.38	110.21
28	a	424	SQD	O47-C7-C8	6.09	124.20	111.55
24	d	404	CLA	C3B-C4B-NB	6.10	117.09	109.21
24	b	603	CLA	C2C-C1C-NC	6.10	114.42	110.22
24	B	602	CLA	O2D-CGD-CBD	6.13	122.25	111.30
28	l	102	SQD	O6-C1-C2	6.13	118.23	108.23
27	A	611	PL9	C7-C3-C2	6.18	132.01	123.23
24	D	404	CLA	C3C-C4C-NC	6.20	116.50	110.21
24	b	602	CLA	O2D-CGD-CBD	6.22	122.42	111.30
28	a	413	SQD	O8-S-C6	6.28	113.68	106.01
24	b	608	CLA	C2C-C1C-NC	6.31	114.56	110.22
24	B	617	CLA	C3C-C4C-NC	6.32	116.61	110.21
24	c	504	CLA	C3B-C4B-NB	6.34	117.40	109.21
40	d	408	DGD	O2G-C1B-C2B	6.37	124.78	111.55
24	C	510	CLA	C3C-C4C-NC	6.43	116.73	110.21
24	a	410	CLA	C3C-C4C-NC	6.46	116.75	110.21
24	c	508	CLA	C3C-C4C-NC	6.49	116.78	110.21
24	C	506	CLA	C3C-C4C-NC	6.54	116.83	110.21
24	B	614	CLA	C3C-C4C-NC	6.58	116.88	110.21
24	A	607	CLA	C3C-C4C-NC	6.58	116.88	110.21
24	d	403	CLA	C2C-C1C-NC	6.60	114.76	110.22
24	C	505	CLA	C3C-C4C-NC	6.60	116.89	110.21
29	B	621	LMG	O7-C10-C11	6.62	125.29	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	C3C-C4C-NC	6.65	116.95	110.21
27	a	412	PL9	C7-C3-C4	6.69	122.31	116.88
24	B	605	CLA	C3C-C4C-NC	6.69	116.99	110.21
31	c	521	LMT	O1B-C4'-C3'	6.72	123.37	107.19
24	D	405	CLA	C3C-C4C-NC	6.72	117.02	110.21
24	b	602	CLA	C3C-C4C-NC	6.77	117.07	110.21
24	B	603	CLA	C3C-C4C-NC	6.77	117.07	110.21
24	c	513	CLA	C3C-C4C-NC	6.78	117.08	110.21
24	B	602	CLA	C3C-C4C-NC	6.79	117.09	110.21
24	B	610	CLA	C3C-C4C-NC	6.83	117.13	110.21
24	B	616	CLA	C3C-C4C-NC	6.84	117.14	110.21
27	A	611	PL9	C3-C4-C5	6.85	127.83	118.63
24	b	609	CLA	C3C-C4C-NC	6.86	117.16	110.21
24	b	614	CLA	C3C-C4C-NC	6.91	117.21	110.21
24	b	611	CLA	C3C-C4C-NC	6.95	117.25	110.21
24	C	511	CLA	C2C-C1C-NC	6.96	115.01	110.22
24	c	506	CLA	C3C-C4C-NC	7.01	117.31	110.21
28	F	104	SQD	O9-S-C6	7.06	112.86	106.83
24	B	609	CLA	C3C-C4C-NC	7.08	117.38	110.21
29	C	519	LMG	O8-C28-C29	7.08	132.50	111.90
28	A	622	SQD	O9-S-C6	7.10	112.89	106.83
28	l	102	SQD	O7-S-C6	7.17	112.96	106.83
24	b	606	CLA	C2C-C1C-NC	7.18	115.16	110.22
24	c	509	CLA	C3C-C4C-NC	7.18	117.48	110.21
24	B	603	CLA	C2C-C1C-NC	7.18	115.16	110.22
24	c	506	CLA	C2C-C1C-NC	7.19	115.17	110.22
24	B	612	CLA	C3C-C4C-NC	7.23	117.54	110.21
24	c	510	CLA	C3C-C4C-NC	7.24	117.55	110.21
24	C	508	CLA	C3C-C4C-NC	7.26	117.57	110.21
28	x	101	SQD	O9-S-C6	7.29	113.06	106.83
24	b	615	CLA	C2C-C1C-NC	7.31	115.25	110.22
24	C	513	CLA	C3C-C4C-NC	7.35	117.66	110.21
38	c	531	HTG	C1'-S1-C1	7.36	111.20	100.28
24	b	606	CLA	C3C-C4C-NC	7.44	117.75	110.21
24	C	512	CLA	C2C-C1C-NC	7.48	115.37	110.22
28	h	105	SQD	O7-S-C6	7.49	113.22	106.83
24	b	607	CLA	C2C-C1C-NC	7.50	115.38	110.22
24	c	510	CLA	C2C-C1C-NC	7.55	115.42	110.22
38	B	624	HTG	C1'-S1-C1	7.59	111.54	100.28
24	C	507	CLA	C3C-C4C-NC	7.61	117.92	110.21
28	b	633	SQD	O9-S-C6	7.62	113.34	106.83
24	C	502	CLA	C2C-C1C-NC	7.62	115.47	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C3C-C4C-NC	7.68	118.00	110.21
40	D	408	DGD	O2G-C1B-C2B	7.72	127.58	111.55
24	C	503	CLA	C2C-C1C-NC	7.82	115.60	110.22
24	A	606	CLA	C2C-C1C-NC	7.82	115.60	110.22
24	b	613	CLA	C2C-C1C-NC	7.87	115.63	110.22
24	b	603	CLA	C3C-C4C-NC	7.87	118.19	110.21
24	C	503	CLA	C3C-C4C-NC	7.90	118.21	110.21
24	B	615	CLA	C2C-C1C-NC	7.90	115.66	110.22
24	C	513	CLA	C2C-C1C-NC	7.93	115.67	110.22
38	C	522	HTG	C1'-S1-C1	7.97	112.10	100.28
24	c	503	CLA	C2C-C1C-NC	7.99	115.71	110.22
24	a	408	CLA	C3C-C4C-NC	8.05	118.37	110.21
24	C	510	CLA	C2C-C1C-NC	8.07	115.77	110.22
24	B	614	CLA	C2C-C1C-NC	8.09	115.78	110.22
24	b	605	CLA	C3C-C4C-NC	8.10	118.41	110.21
28	x	101	SQD	O8-S-C6	8.11	115.92	106.01
24	C	501	CLA	O2D-CGD-CBD	8.22	126.00	111.30
31	M	102	LMT	C1-O1'-C1'	8.27	128.06	113.87
24	B	611	CLA	C2C-C1C-NC	8.28	115.91	110.22
28	F	104	SQD	O6-C1-C2	8.30	121.78	108.23
24	c	505	CLA	C2C-C1C-NC	8.32	115.95	110.22
24	b	617	CLA	C3C-C4C-NC	8.40	118.72	110.21
28	a	413	SQD	O9-S-C6	8.41	114.02	106.83
24	d	405	CLA	C2C-C1C-NC	8.47	116.05	110.22
28	A	612	SQD	O9-S-C6	8.49	114.08	106.83
40	d	408	DGD	O3G-C1D-C2D	8.49	122.09	108.23
24	B	606	CLA	C3C-C4C-NC	8.50	118.82	110.21
24	b	613	CLA	C3C-C4C-NC	8.51	118.83	110.21
24	b	602	CLA	C2C-C1C-NC	8.64	116.16	110.22
24	b	610	CLA	C3C-C4C-NC	8.64	118.96	110.21
24	c	509	CLA	C2C-C1C-NC	8.67	116.19	110.22
28	a	413	SQD	O6-C1-C2	8.72	122.46	108.23
24	b	610	CLA	C2C-C1C-NC	8.83	116.29	110.22
24	a	407	CLA	C2C-C1C-NC	8.88	116.33	110.22
24	B	606	CLA	C2C-C1C-NC	8.95	116.38	110.22
24	b	614	CLA	C2C-C1C-NC	8.96	116.38	110.22
24	D	405	CLA	C2C-C1C-NC	8.98	116.40	110.22
24	c	507	CLA	C2C-C1C-NC	9.03	116.43	110.22
24	c	505	CLA	C3C-C4C-NC	9.07	119.40	110.21
24	A	607	CLA	C2C-C1C-NC	9.13	116.50	110.22
24	b	604	CLA	C2C-C1C-NC	9.21	116.56	110.22
24	C	508	CLA	C2C-C1C-NC	9.23	116.57	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	C2C-C1C-NC	9.23	116.57	110.22
24	B	617	CLA	C2C-C1C-NC	9.29	116.61	110.22
24	B	605	CLA	C2C-C1C-NC	9.30	116.61	110.22
24	c	502	CLA	C2C-C1C-NC	9.30	116.62	110.22
24	a	408	CLA	C2C-C1C-NC	9.32	116.63	110.22
24	B	602	CLA	C2C-C1C-NC	9.36	116.66	110.22
24	c	511	CLA	C2C-C1C-NC	9.50	116.75	110.22
24	B	609	CLA	C2C-C1C-NC	9.63	116.84	110.22
24	A	609	CLA	C2C-C1C-NC	9.66	116.86	110.22
24	b	617	CLA	C2C-C1C-NC	9.69	116.89	110.22
24	b	612	CLA	C2C-C1C-NC	9.73	116.91	110.22
24	D	404	CLA	C2C-C1C-NC	9.74	116.92	110.22
28	a	424	SQD	O9-S-C6	9.78	115.18	106.83
24	C	507	CLA	C2C-C1C-NC	9.81	116.97	110.22
24	a	410	CLA	C2C-C1C-NC	9.84	116.99	110.22
24	B	607	CLA	C2C-C1C-NC	9.85	116.99	110.22
24	C	509	CLA	C2C-C1C-NC	9.98	117.08	110.22
24	B	604	CLA	C2C-C1C-NC	10.12	117.18	110.22
24	c	512	CLA	C2C-C1C-NC	10.15	117.20	110.22
24	b	616	CLA	C2C-C1C-NC	10.16	117.21	110.22
24	b	611	CLA	C2C-C1C-NC	10.24	117.26	110.22
24	C	506	CLA	C2C-C1C-NC	10.29	117.30	110.22
24	B	616	CLA	C2C-C1C-NC	10.34	117.33	110.22
24	D	403	CLA	C2C-C1C-NC	10.34	117.33	110.22
24	c	508	CLA	C2C-C1C-NC	10.42	117.39	110.22
24	c	504	CLA	C2C-C1C-NC	10.50	117.44	110.22
24	B	608	CLA	C2C-C1C-NC	10.56	117.48	110.22
38	C	529	HTG	C1'-S1-C1	10.64	116.06	100.28
24	b	609	CLA	C2C-C1C-NC	10.67	117.56	110.22
24	C	504	CLA	C2C-C1C-NC	10.79	117.64	110.22
24	C	505	CLA	C2C-C1C-NC	10.84	117.67	110.22
24	b	605	CLA	C2C-C1C-NC	10.95	117.75	110.22
24	c	501	CLA	C2C-C1C-NC	11.04	117.82	110.22
41	E	113	HEM	CAD-CBD-CGD	11.22	131.84	112.66
24	B	612	CLA	C2C-C1C-NC	11.28	117.98	110.22
24	C	501	CLA	C2C-C1C-NC	11.54	118.16	110.22
24	d	404	CLA	C2C-C1C-NC	11.72	118.28	110.22
24	B	610	CLA	C2C-C1C-NC	11.94	118.43	110.22

All (207) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
24	b	613	CLA	NC
24	b	613	CLA	ND
24	b	613	CLA	NA
24	c	508	CLA	NC
24	c	508	CLA	ND
24	c	508	CLA	NA
24	c	507	CLA	NC
24	c	507	CLA	ND
24	c	507	CLA	NA
24	C	501	CLA	NC
24	C	501	CLA	ND
24	C	501	CLA	NA
24	b	603	CLA	NC
24	b	603	CLA	NA
24	b	603	CLA	ND
24	b	614	CLA	NC
24	b	614	CLA	ND
24	b	614	CLA	NA
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	b	611	CLA	NC
24	b	611	CLA	ND
24	b	611	CLA	NA
24	C	506	CLA	NC
24	C	506	CLA	ND
24	C	506	CLA	NA
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	c	511	CLA	NC
24	c	511	CLA	ND
24	c	511	CLA	NA
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	513	CLA	NA
24	c	501	CLA	NC
24	c	501	CLA	ND
24	c	501	CLA	NA
24	D	404	CLA	NC
24	D	404	CLA	NA

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Mol	Chain	Res	Type	Atom
24	D	404	CLA	ND
24	B	610	CLA	NC
24	B	610	CLA	ND
24	B	610	CLA	NA
24	c	512	CLA	NC
24	c	512	CLA	ND
24	c	512	CLA	NA
24	c	502	CLA	NC
24	c	502	CLA	ND
24	c	502	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	ND
24	B	608	CLA	NA
24	C	507	CLA	NC
24	C	507	CLA	NA
24	b	616	CLA	NC
24	b	616	CLA	NA
24	b	609	CLA	NC
24	b	609	CLA	ND
24	b	609	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	B	617	CLA	NC
24	B	617	CLA	ND
24	B	617	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	ND
24	b	612	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	NA
24	B	604	CLA	ND
24	b	615	CLA	NC
24	b	615	CLA	ND
24	b	615	CLA	NA
24	b	602	CLA	NC

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Mol	Chain	Res	Type	Atom
24	b	602	CLA	ND
24	b	602	CLA	NA
24	C	504	CLA	NC
24	C	504	CLA	ND
24	C	504	CLA	NA
24	d	403	CLA	NC
24	d	403	CLA	ND
24	d	403	CLA	NA
24	c	510	CLA	NC
24	c	510	CLA	ND
24	c	510	CLA	NA
24	C	511	CLA	NC
24	C	511	CLA	ND
24	C	511	CLA	NA
24	b	605	CLA	NC
24	b	605	CLA	ND
24	b	605	CLA	NA
24	a	410	CLA	NC
24	a	410	CLA	ND
24	a	410	CLA	NA
24	b	617	CLA	NC
24	b	617	CLA	ND
24	b	617	CLA	NA
24	A	609	CLA	NC
24	A	609	CLA	ND
24	A	609	CLA	NA
24	c	506	CLA	NC
24	c	506	CLA	ND
24	c	506	CLA	NA
24	B	612	CLA	NC
24	B	612	CLA	ND
24	B	612	CLA	NA
24	B	603	CLA	NC
24	B	603	CLA	ND
24	B	603	CLA	NA
24	C	503	CLA	NC
24	C	503	CLA	ND
24	C	503	CLA	NA
24	c	509	CLA	NC
24	c	509	CLA	ND
24	c	509	CLA	NA
24	B	609	CLA	NC

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Mol	Chain	Res	Type	Atom
24	B	609	CLA	ND
24	B	609	CLA	NA
24	b	604	CLA	NC
24	b	604	CLA	NA
24	b	604	CLA	ND
24	A	607	CLA	NC
24	A	607	CLA	ND
24	A	607	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	B	615	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	ND
24	C	509	CLA	NA
24	c	503	CLA	NC
24	c	503	CLA	ND
24	c	503	CLA	NA
24	B	602	CLA	NC
24	B	602	CLA	ND
24	B	602	CLA	NA
24	d	404	CLA	NC
24	d	404	CLA	NA
24	d	404	CLA	ND
24	B	607	CLA	NC
24	B	607	CLA	NA
24	B	607	CLA	ND
24	c	504	CLA	NC
24	c	504	CLA	ND
24	c	504	CLA	NA
24	c	505	CLA	NC
24	c	505	CLA	NA
24	c	505	CLA	ND
24	C	512	CLA	NC
24	C	512	CLA	ND
24	C	512	CLA	NA
24	c	513	CLA	NC
24	c	513	CLA	ND
24	c	513	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	NA
24	A	606	CLA	NC
24	A	606	CLA	ND

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Mol	Chain	Res	Type	Atom
24	A	606	CLA	NA
24	b	607	CLA	NC
24	b	607	CLA	NA
24	b	607	CLA	ND
24	C	505	CLA	NC
24	C	505	CLA	NA
24	C	505	CLA	ND
24	d	405	CLA	NC
24	d	405	CLA	ND
24	d	405	CLA	NA
24	a	408	CLA	NC
24	a	408	CLA	ND
24	a	408	CLA	NA
24	D	403	CLA	NC
24	D	403	CLA	ND
24	D	403	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	D	405	CLA	NC
24	D	405	CLA	ND
24	D	405	CLA	NA
24	b	608	CLA	NC
24	b	608	CLA	ND
24	b	608	CLA	NA
24	b	606	CLA	NC
24	b	606	CLA	NA
24	b	606	CLA	ND
24	C	502	CLA	NC
24	C	502	CLA	ND
24	C	502	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	a	407	CLA	NC
24	a	407	CLA	ND
24	a	407	CLA	NA

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	d	408	DGD	C2G-O2G-C1B-C2B
29	d	412	LMG	C8-O7-C10-C11
40	D	408	DGD	C2G-O2G-C1B-O1B
40	D	408	DGD	C2G-O2G-C1B-C2B

There are no ring outliers.

94 monomers are involved in 234 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	606	CLA	4	0
24	A	607	CLA	2	0
25	A	608	PHO	2	0
24	A	609	CLA	2	0
26	A	610	BCR	3	0
27	A	611	PL9	6	0
28	A	612	SQD	2	0
29	A	613	LMG	3	0
30	A	614	GOL	1	0
30	A	615	GOL	3	0
28	A	616	SQD	1	0
28	A	622	SQD	2	0
24	B	602	CLA	12	0
24	B	603	CLA	1	0
24	B	604	CLA	3	0
24	B	605	CLA	2	0
24	B	606	CLA	3	0
24	B	607	CLA	3	0
24	B	608	CLA	2	0
24	B	609	CLA	1	0
24	B	610	CLA	4	0
24	B	611	CLA	3	0
24	B	612	CLA	2	0
24	B	613	CLA	4	0
24	B	614	CLA	3	0
24	B	615	CLA	4	0
24	B	616	CLA	1	0
24	B	617	CLA	2	0
26	B	618	BCR	4	0
26	B	619	BCR	4	0
26	B	620	BCR	6	0
29	B	621	LMG	3	0
31	B	622	LMT	2	0
38	B	623	HTG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	629	GOL	1	0
29	B	634	LMG	6	0
34	B	646	PGE	2	0
35	B	652	P6G	1	0
24	C	501	CLA	3	0
24	C	502	CLA	4	0
24	C	503	CLA	2	0
24	C	504	CLA	3	0
24	C	505	CLA	4	0
24	C	506	CLA	4	0
24	C	507	CLA	3	0
24	C	508	CLA	2	0
24	C	509	CLA	3	0
24	C	510	CLA	4	0
24	C	511	CLA	4	0
24	C	512	CLA	3	0
24	C	513	CLA	2	0
26	C	514	BCR	2	0
26	C	515	BCR	4	0
29	C	519	LMG	1	0
38	C	521	HTG	1	0
30	C	523	GOL	3	0
26	C	525	BCR	1	0
29	C	526	LMG	3	0
30	C	528	GOL	10	0
38	C	529	HTG	1	0
38	C	531	HTG	1	0
38	C	532	HTG	1	0
35	C	541	P6G	3	0
25	D	401	PHO	3	0
30	D	402	GOL	1	0
24	D	403	CLA	3	0
24	D	404	CLA	2	0
24	D	405	CLA	5	0
26	D	406	BCR	4	0
40	D	408	DGD	2	0
32	D	409	LHG	1	0
32	D	411	LHG	1	0
30	D	412	GOL	1	0
36	D	419	EDO	3	0
32	E	101	LHG	2	0
41	E	113	HEM	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	H	101	HTG	1	0
26	H	102	BCR	3	0
33	H	106	PG4	4	0
31	I	101	LMT	1	0
33	I	104	PG4	2	0
31	J	103	LMT	1	0
26	K	101	BCR	6	0
31	M	101	LMT	1	0
30	O	305	GOL	2	0
34	O	308	PGE	5	0
30	T	101	GOL	1	0
26	T	102	BCR	9	0
30	T	103	GOL	1	0
35	T	105	P6G	2	0
30	U	201	GOL	2	0
43	V	216	2PE	3	0
31	Y	101	LMT	1	0
40	d	408	DGD	0	1

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.86	2 (0%) 89 90	16, 22, 46, 78	0
1	a	334/344 (97%)	-0.82	3 (0%) 84 86	17, 24, 52, 89	0
2	B	504/506 (99%)	-0.63	18 (3%) 43 47	17, 26, 57, 92	0
2	b	506/506 (100%)	-0.49	29 (5%) 24 28	19, 29, 71, 129	0
3	C	451/458 (98%)	-0.75	4 (0%) 84 86	19, 31, 46, 87	0
3	c	458/458 (100%)	-0.61	12 (2%) 56 60	24, 35, 51, 108	0
4	D	341/342 (99%)	-0.88	4 (1%) 79 82	16, 23, 40, 114	0
4	d	341/342 (99%)	-0.82	5 (1%) 74 77	18, 26, 44, 110	0
5	E	81/83 (97%)	-0.23	4 (4%) 30 34	26, 41, 66, 92	0
5	e	81/83 (97%)	0.25	8 (9%) 8 9	32, 46, 75, 118	0
6	F	34/44 (77%)	-0.36	3 (8%) 11 12	26, 33, 63, 82	0
6	f	32/44 (72%)	-0.21	3 (9%) 9 10	30, 38, 78, 117	0
7	H	65/65 (100%)	-0.43	4 (6%) 21 24	23, 33, 47, 123	0
7	h	65/65 (100%)	-0.23	3 (4%) 33 37	26, 38, 56, 116	0
8	I	37/38 (97%)	-0.35	3 (8%) 13 14	28, 35, 75, 91	0
8	i	37/38 (97%)	-0.38	2 (5%) 26 30	27, 34, 67, 89	0
9	J	39/40 (97%)	-0.29	6 (15%) 2 2	24, 36, 108, 130	0
9	j	39/40 (97%)	-0.24	5 (12%) 4 4	29, 43, 75, 89	0
10	K	37/37 (100%)	-0.54	0 100 100	31, 37, 56, 70	0
10	k	37/37 (100%)	-0.47	0 100 100	36, 44, 64, 75	0
11	L	37/37 (100%)	-0.45	3 (8%) 13 14	15, 21, 70, 92	0
11	l	37/37 (100%)	-0.33	4 (10%) 6 7	18, 22, 70, 95	0
12	M	33/36 (91%)	-0.59	2 (6%) 22 25	19, 22, 44, 88	0
12	m	34/36 (94%)	-0.48	3 (8%) 11 12	20, 24, 75, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	245/245 (100%)	-0.11	15 (6%) 22 25	18, 33, 69, 128	0
13	o	245/245 (100%)	0.04	25 (10%) 7 8	21, 34, 84, 136	0
14	T	29/32 (90%)	-0.66	2 (6%) 18 20	18, 23, 47, 101	0
14	t	29/32 (90%)	-0.81	1 (3%) 46 49	19, 23, 44, 81	0
15	U	97/104 (93%)	-0.53	2 (2%) 64 67	21, 31, 58, 95	0
15	u	97/104 (93%)	-0.58	1 (1%) 82 84	24, 31, 47, 84	0
16	V	137/137 (100%)	-0.76	0 100 100	20, 29, 46, 66	0
16	v	137/137 (100%)	-0.49	4 (2%) 52 56	26, 38, 58, 73	0
17	Y	29/30 (96%)	1.36	6 (20%) 1 1	36, 49, 76, 109	0
17	y	29/30 (96%)	1.19	6 (20%) 1 1	46, 60, 81, 92	0
18	X	40/41 (97%)	0.25	4 (10%) 8 9	30, 40, 100, 118	0
18	x	40/41 (97%)	0.29	6 (15%) 3 3	36, 43, 112, 132	0
19	Z	62/62 (100%)	0.23	8 (12%) 4 4	37, 47, 86, 94	0
19	z	62/62 (100%)	0.81	14 (22%) 1 1	50, 62, 101, 117	0
All	All	5272/5362 (98%)	-0.51	224 (4%) 37 40	15, 30, 65, 136	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	2	ALA	13.7
7	h	66	GLY	13.4
13	o	3	ALA	13.1
13	O	2	ALA	12.8
17	Y	19	ILE	12.0
13	O	3	ALA	10.7
17	Y	18	VAL	10.6
18	x	40	SER	9.4
18	X	1	MET	9.3
12	m	35	SER	9.1
17	y	18	VAL	8.1
19	z	3	ILE	8.0
7	H	65	LEU	8.0
17	y	19	ILE	7.8
2	b	507	ASP	7.8
13	O	58	ASN	7.8
3	c	17	ALA	7.7
18	X	40	SER	7.7

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Mol	Chain	Res	Type	RSRZ
18	x	1	MET	7.7
5	e	5	THR	7.4
2	b	495	PHE	7.3
5	e	4	THR	7.2
19	Z	3	ILE	6.9
13	o	25	THR	6.8
7	h	65	LEU	6.6
2	b	506	SER	6.6
6	f	14	PRO	6.6
13	o	60	ARG	6.6
3	c	18	ALA	6.5
4	d	11	GLU	6.5
2	b	505	ARG	6.5
14	T	30	THR	6.4
9	J	2	GLU	6.2
2	b	485	GLU	6.1
5	E	84	LYS	6.1
2	b	488	PRO	6.0
13	o	246	ALA	5.9
18	X	38	GLN	5.9
19	z	60	PHE	5.9
12	M	34	LYS	5.7
2	B	485	GLU	5.7
17	y	20	ALA	5.7
17	Y	22	LEU	5.7
13	O	62	GLU	5.7
13	o	62	GLU	5.5
2	b	502	VAL	5.5
19	z	62	VAL	5.5
12	M	33	GLN	5.4
13	o	4	THR	5.3
19	Z	31	GLN	5.3
13	O	56	PRO	5.3
19	z	31	GLN	5.2
2	b	503	THR	5.2
18	x	38	GLN	5.2
13	O	4	THR	5.1
2	b	489	GLU	5.1
5	e	84	LYS	5.1
13	o	35	SER	5.1
11	L	1	MET	5.0
5	E	4	THR	5.0

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Mol	Chain	Res	Type	RSRZ
3	C	23	ALA	4.8
19	z	1	MET	4.8
18	X	2	THR	4.7
9	j	6	GLY	4.7
13	O	61	GLN	4.7
19	z	32	ASP	4.7
17	Y	20	ALA	4.7
11	L	2	GLU	4.7
2	B	495	PHE	4.6
1	a	11	ALA	4.6
2	B	494	GLY	4.5
11	l	1	MET	4.5
11	l	3	PRO	4.5
13	o	59	LYS	4.4
2	B	502	VAL	4.4
2	b	127	ARG	4.4
4	D	11	GLU	4.4
5	e	6	GLY	4.3
13	o	27	ARG	4.3
2	b	486	LEU	4.3
5	e	61	ARG	4.3
12	m	34	LYS	4.3
19	z	4	LEU	4.2
3	c	21	ILE	4.2
18	x	2	THR	4.2
3	c	19	ASN	4.2
9	J	6	GLY	4.2
6	f	16	PHE	4.2
16	v	15	GLU	4.1
13	O	25	THR	4.1
4	D	238	THR	4.1
11	l	2	GLU	4.1
1	A	11	ALA	4.1
17	Y	43	ARG	4.1
15	u	8	GLU	4.1
2	b	484	PRO	4.0
19	Z	30	PRO	4.0
19	z	34	ASP	4.0
15	U	8	GLU	4.0
4	d	238	THR	4.0
17	y	22	LEU	4.0
13	o	36	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
5	e	25	ILE	3.9
13	O	89	SER	3.9
3	C	24	THR	3.9
8	i	36	ASP	3.9
7	H	64	ALA	3.8
2	b	487	SER	3.8
4	D	12	ARG	3.8
13	O	60	ARG	3.8
19	Z	32	ASP	3.7
8	I	36	ASP	3.7
13	o	26	ALA	3.6
13	o	61	GLN	3.6
9	J	3	SER	3.6
2	b	86	ILE	3.6
2	b	85	GLY	3.6
6	F	12	SER	3.6
9	j	5	GLY	3.6
17	y	41	VAL	3.6
3	c	207	ARG	3.5
2	B	505	ARG	3.5
13	o	58	ASN	3.5
9	j	4	GLU	3.5
13	o	23	ASP	3.5
12	m	33	GLN	3.5
4	D	240	ALA	3.4
8	I	34	ARG	3.4
18	x	37	VAL	3.4
2	B	503	THR	3.4
7	H	66	GLY	3.3
13	O	207	ARG	3.3
17	y	43	ARG	3.3
7	h	64	ALA	3.3
2	b	496	TYR	3.3
2	B	489	GLU	3.2
2	B	487	SER	3.2
19	z	61	VAL	3.2
1	a	262	TYR	3.2
13	o	56	PRO	3.2
2	b	494	GLY	3.2
6	F	16	PHE	3.2
6	F	13	TYR	3.2
2	b	293	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
19	Z	35	ARG	3.1
14	t	30	THR	3.1
16	v	106	ASN	3.1
11	L	3	PRO	3.0
9	J	4	GLU	3.0
9	J	5	GLY	3.0
4	d	237	PRO	3.0
19	z	35	ARG	2.9
2	b	294	SER	2.9
2	b	492	GLU	2.9
2	b	497	GLN	2.9
9	J	7[A]	ARG	2.9
19	z	30	PRO	2.9
18	x	39	ARG	2.9
13	o	24	ASP	2.8
2	B	492	GLU	2.8
13	O	59	LYS	2.8
4	d	236	ASN	2.8
13	o	207	ARG	2.7
3	C	191	PRO	2.7
19	z	33	TRP	2.7
2	b	295	GLY	2.7
13	O	24	ASP	2.7
5	E	6	GLY	2.6
13	o	34	SER	2.6
13	o	211	ILE	2.6
2	b	84	THR	2.6
2	B	295	GLY	2.6
19	z	42	LEU	2.6
2	b	504	THR	2.6
19	z	7	LEU	2.5
5	E	81	GLU	2.5
13	o	132	ASN	2.5
3	c	22	PHE	2.5
19	Z	1	MET	2.5
3	c	191	PRO	2.5
19	Z	34	ASP	2.5
1	a	12	ASN	2.5
2	B	501	ASP	2.4
3	c	106	VAL	2.4
2	B	488	PRO	2.4
2	B	85	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	484	PRO	2.4
15	U	65	PRO	2.4
13	o	57	LYS	2.4
2	B	504	THR	2.4
2	b	128	THR	2.4
19	Z	38	GLN	2.4
13	O	63	ALA	2.3
8	i	34	ARG	2.3
9	j	7	ARG	2.3
16	v	17	LYS	2.3
5	e	81	GLU	2.3
13	O	23	ASP	2.3
3	C	207	ARG	2.3
2	b	499	VAL	2.3
2	b	374	ASN	2.3
2	b	373	LYS	2.3
17	Y	21	GLN	2.2
9	j	2	GLU	2.2
5	e	62[A]	SER	2.2
1	A	243	GLU	2.2
13	o	33	ASP	2.2
2	B	293	ALA	2.2
4	d	240	ALA	2.2
8	I	38	GLU	2.2
16	v	16	GLY	2.2
13	o	89	SER	2.2
3	c	16	GLU	2.2
3	c	20	SER	2.1
2	b	130[A]	GLU	2.1
3	c	142	GLU	2.1
2	B	486	LEU	2.1
13	o	28	GLY	2.1
6	f	15	ILE	2.1
14	T	29	ILE	2.1
11	l	5	PRO	2.1
7	H	6	TRP	2.0
2	B	483	ASP	2.0
3	c	462[A]	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
12	FME	m	1[A]	10/11	0.97	0.10	-	24,30,61,84	7
8	FME	i	1	10/11	0.99	0.06	-	30,33,36,37	0
12	FME	M	1	10/11	0.98	0.07	-	27,32,64,68	0
14	FME	T	1[B]	10/11	0.99	0.07	-	21,25,32,35	7
12	FME	m	1[B]	10/11	0.97	0.10	-	30,33,55,66	7
14	FME	T	1[A]	10/11	0.99	0.07	-	21,25,47,47	7
14	FME	t	1[A]	10/11	0.98	0.07	-	20,24,39,42	7
4	MHS	d	336	11/12	0.99	0.05	-	27,32,44,44	0
14	FME	t	1[B]	10/11	0.98	0.07	-	20,24,31,36	7
8	FME	I	1	10/11	0.98	0.05	-	26,32,40,44	0
4	MHS	D	336	11/12	0.98	0.07	-	23,28,37,38	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	PG4	B	642	13/13	0.77	0.47	60.06	66,86,115,120	0
28	SQD	h	105	54/54	0.51	0.45	36.39	76,100,195,214	0
31	LMT	J	103	35/35	0.72	0.27	27.78	47,78,115,134	0
34	PGE	o	306	10/10	0.81	0.46	27.71	70,92,102,103	0
38	HTG	h	101	19/19	0.67	0.28	23.43	62,86,123,141	0
30	GOL	c	529	6/6	0.93	0.33	22.79	27,31,39,40	6
35	P6G	E	110	19/19	0.79	0.46	21.91	49,95,111,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	PG4	E	102	13/13	0.79	0.36	21.70	62,81,106,120	0
34	PGE	O	308	10/10	0.94	0.29	19.82	31,62,83,96	0
40	DGD	D	408	66/66	0.67	0.29	17.63	56,88,142,175	0
34	PGE	o	309	10/10	0.88	0.35	16.33	53,78,92,97	0
33	PG4	B	637	13/13	0.78	0.18	16.10	68,82,106,106	0
30	GOL	C	528	6/6	0.95	0.27	15.96	24,27,36,38	6
33	PG4	C	535	13/13	0.84	0.33	14.46	66,74,108,121	0
34	PGE	V	215	10/10	0.77	0.50	13.83	66,90,103,111	0
39	1PE	V	217	16/16	0.69	0.55	13.54	63,93,120,133	0
33	PG4	J	105	13/13	0.71	0.36	12.99	75,88,110,115	0
34	PGE	c	539	10/10	0.74	0.49	12.43	80,90,104,104	0
34	PGE	E	109	10/10	0.87	0.33	12.13	51,93,103,106	0
34	PGE	B	648	10/10	0.88	0.21	11.87	55,75,82,93	0
31	LMT	t	103	35/35	0.80	0.22	11.52	32,75,110,117	0
34	PGE	V	214	10/10	0.81	0.43	11.46	50,86,96,98	0
33	PG4	V	210	13/13	0.81	0.39	11.22	53,84,115,120	0
35	P6G	B	652	19/19	0.90	0.27	10.62	42,84,105,109	0
39	1PE	B	654	16/16	0.89	0.22	10.51	46,68,92,105	0
33	PG4	x	102	13/13	0.85	0.48	9.91	79,95,107,108	0
33	PG4	X	102	13/13	0.79	0.27	9.56	77,95,113,114	0
34	PGE	O	309	10/10	0.77	0.48	9.04	62,86,111,111	0
31	LMT	F	102	35/35	0.82	0.28	8.87	43,81,105,126	0
31	LMT	m	101	35/35	0.79	0.20	8.82	45,62,75,92	0
31	LMT	a	401	35/35	0.86	0.16	8.81	37,52,75,83	0
31	LMT	u	203	35/35	0.72	0.39	8.78	42,77,115,137	0
40	DGD	d	408	66/66	0.79	0.35	8.28	57,89,155,184	0
33	PG4	e	104	13/13	0.75	0.49	8.21	78,94,120,120	0
33	PG4	X	101	13/13	0.84	0.35	8.11	63,89,105,108	0
33	PG4	K	102	13/13	0.72	0.25	7.76	56,70,102,109	0
38	HTG	a	418	19/19	0.76	0.27	7.74	53,84,123,124	0
30	GOL	O	305	6/6	0.89	0.34	7.60	55,65,71,77	0
33	PG4	V	209	13/13	0.92	0.26	7.58	51,84,95,101	0
33	PG4	b	636	13/13	0.86	0.21	7.49	71,79,90,93	0
30	GOL	D	413	6/6	0.95	0.21	7.40	58,67,76,84	0
38	HTG	C	529	19/19	0.47	0.27	7.34	70,102,136,144	0
38	HTG	H	101	19/19	0.65	0.24	7.22	50,94,122,122	0
31	LMT	f	101	35/35	0.84	0.27	7.06	54,85,110,119	0
30	GOL	c	528	6/6	0.95	0.21	6.53	78,79,88,89	0
31	LMT	A	617	35/35	0.92	0.15	6.53	37,55,92,105	0
33	PG4	a	421	13/13	0.92	0.09	6.50	76,89,99,102	0
38	HTG	V	204	19/19	0.95	0.27	6.44	36,52,89,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	P6G	A	623	19/19	0.84	0.18	6.09	48,60,95,96	0
34	PGE	T	104	7/10	0.96	0.10	6.02	76,77,96,103	0
33	PG4	H	107	13/13	0.82	0.21	5.99	68,83,105,110	0
30	GOL	B	635	6/6	0.89	0.28	5.75	46,67,79,83	0
36	EDO	B	656	4/4	0.79	0.43	5.71	78,87,100,107	0
33	PG4	j	104	13/13	0.76	0.24	5.69	78,97,113,116	0
39	1PE	e	105	16/16	0.85	0.21	5.66	77,93,116,121	0
30	GOL	c	525	6/6	0.98	0.20	5.64	47,49,64,80	0
33	PG4	c	534	13/13	0.89	0.28	5.52	69,85,99,112	0
34	PGE	C	539	10/10	0.95	0.23	5.38	56,73,94,96	0
34	PGE	t	105	7/10	0.95	0.12	5.34	58,79,84,87	0
28	SQD	A	616	54/54	0.90	0.13	5.26	39,65,102,107	0
34	PGE	B	649	10/10	0.81	0.24	5.07	66,82,101,105	0
34	PGE	E	104	10/10	0.92	0.12	5.04	67,76,99,106	0
35	P6G	A	624	19/19	0.90	0.11	5.04	70,85,105,113	0
30	GOL	O	306	6/6	0.96	0.13	4.89	39,45,55,97	0
43	2PE	V	216	28/28	0.76	0.36	4.85	44,91,110,123	0
33	PG4	c	532	13/13	0.91	0.19	4.79	70,78,98,101	0
29	LMG	d	412	55/55	0.73	0.25	4.77	47,77,119,137	0
38	HTG	C	522	19/19	0.85	0.24	4.73	50,83,100,110	0
30	GOL	a	416	6/6	0.95	0.12	4.54	39,57,72,77	0
30	GOL	O	304	6/6	0.90	0.36	4.52	60,69,79,88	0
30	GOL	D	402	6/6	0.97	0.11	4.49	31,37,43,44	0
30	GOL	u	202	6/6	0.91	0.22	4.49	50,56,61,63	0
32	LHG	A	618	42/49	0.85	0.22	4.34	49,90,145,167	0
29	LMG	B	634	55/55	0.81	0.19	4.22	39,69,141,167	0
29	LMG	C	526	55/55	0.81	0.23	4.16	47,83,115,124	0
30	GOL	b	629	6/6	0.96	0.14	4.10	36,42,45,50	0
30	GOL	U	201	6/6	0.94	0.24	4.05	40,67,78,98	0
28	SQD	a	417	54/54	0.92	0.10	4.05	40,64,93,101	0
38	HTG	c	523	19/19	0.85	0.31	3.99	65,86,104,106	0
30	GOL	C	523	6/6	0.95	0.17	3.99	35,46,56,62	0
27	PL9	A	611	55/55	0.91	0.13	3.98	39,63,96,107	0
34	PGE	b	638	10/10	0.88	0.18	3.88	55,77,90,93	0
33	PG4	A	619	13/13	0.83	0.22	3.88	83,96,112,112	0
34	PGE	b	643	10/10	0.89	0.21	3.87	70,85,103,116	0
33	PG4	V	211	13/13	0.80	0.39	3.75	54,89,114,120	0
28	SQD	l	102	54/54	0.87	0.14	3.62	46,71,104,172	0
23	BCT	m	104[B]	4/4	0.98	0.11	3.57	7,13,18,19	4
30	GOL	v	207	6/6	0.92	0.32	3.53	63,73,86,86	0
33	PG4	c	533	13/13	0.67	0.38	3.48	77,90,105,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	P6G	d	416	19/19	0.84	0.17	3.47	43,61,100,111	0
30	GOL	A	615	6/6	0.93	0.11	3.45	34,54,62,66	0
28	SQD	F	104	54/54	0.86	0.26	3.32	55,80,110,135	0
33	PG4	i	102	13/13	0.86	0.24	3.31	65,71,81,82	0
23	BCT	m	104[A]	4/4	0.98	0.11	3.31	18,34,38,38	4
29	LMG	z	101	55/55	0.81	0.21	3.26	49,95,120,160	0
38	HTG	c	531	19/19	0.70	0.30	3.25	59,99,122,124	0
34	PGE	i	105	10/10	0.85	0.23	3.25	70,81,89,92	0
35	P6G	d	415	19/19	0.92	0.12	3.20	51,64,88,97	0
29	LMG	A	613	51/55	0.90	0.13	3.20	45,60,82,95	0
34	PGE	c	540	10/10	0.66	0.42	3.19	82,92,110,113	0
29	LMG	a	414	51/55	0.90	0.13	3.18	42,64,80,90	0
33	PG4	I	102	13/13	0.94	0.19	3.18	62,73,97,112	0
36	EDO	X	104	4/4	0.78	0.25	3.09	73,80,83,88	0
31	LMT	M	102	35/35	0.86	0.17	3.06	43,59,82,96	0
29	LMG	C	520	51/55	0.86	0.20	2.98	38,79,108,121	0
36	EDO	E	112	4/4	0.86	0.16	2.98	84,94,96,100	0
33	PG4	U	202	13/13	0.86	0.32	2.80	52,80,100,102	0
34	PGE	B	645	10/10	0.81	0.36	2.78	68,81,89,93	0
35	P6G	T	105	19/19	0.95	0.10	2.71	42,59,85,88	0
33	PG4	C	536	13/13	0.71	0.24	2.70	66,72,93,103	0
36	EDO	O	311	4/4	0.97	0.22	2.58	42,54,57,72	0
33	PG4	B	639	13/13	0.84	0.21	2.57	64,79,104,115	0
35	P6G	j	106	19/19	0.94	0.09	2.50	50,74,98,112	0
30	GOL	t	101	6/6	0.95	0.15	2.50	44,49,56,62	0
29	LMG	b	621	51/55	0.97	0.08	2.49	28,39,53,103	0
30	GOL	v	203	6/6	0.85	0.17	2.44	66,79,82,98	0
34	PGE	C	540	10/10	0.87	0.25	2.38	74,83,102,111	0
30	GOL	d	402	6/6	0.97	0.08	2.34	35,39,45,48	0
30	GOL	V	206	6/6	0.98	0.16	2.33	33,35,42,42	0
35	P6G	D	417	19/19	0.96	0.09	2.30	35,56,89,111	0
27	PL9	a	412	55/55	0.93	0.12	2.29	46,69,101,108	0
30	GOL	B	625	6/6	0.97	0.07	2.28	32,36,38,50	0
32	LHG	D	411	49/49	0.98	0.08	2.25	23,31,81,89	0
31	LMT	j	103	35/35	0.40	0.44	2.19	68,114,162,168	0
31	LMT	c	521	35/35	0.92	0.26	2.16	54,77,95,101	0
40	DGD	C	518	62/66	0.98	0.07	2.16	20,30,71,80	0
24	CLA	b	602	65/65	0.93	0.13	2.12	28,47,99,111	0
32	LHG	a	419	41/49	0.89	0.20	2.10	52,85,176,193	0
33	PG4	J	104	13/13	0.69	0.37	2.10	74,82,107,108	0
28	SQD	A	622	54/54	0.78	0.27	2.03	63,85,136,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	GOL	f	103	6/6	0.97	0.11	1.95	50,53,56,56	0
28	SQD	b	633	54/54	0.89	0.13	1.94	46,66,104,116	0
38	HTG	O	303	19/19	0.97	0.07	1.81	27,31,50,65	0
30	GOL	T	101	6/6	0.97	0.12	1.79	52,52,56,59	0
33	PG4	V	212	13/13	0.78	0.29	1.79	82,96,120,123	0
38	HTG	b	632	19/19	0.78	0.20	1.74	49,79,119,135	0
40	DGD	h	104	62/66	0.96	0.08	1.72	25,35,49,55	0
30	GOL	A	614	6/6	0.97	0.09	1.72	33,37,38,44	0
30	GOL	V	207	6/6	0.96	0.13	1.71	44,49,52,55	0
24	CLA	C	509	65/65	0.98	0.09	1.69	27,33,50,57	0
38	HTG	o	301	19/19	0.97	0.08	1.61	25,32,41,63	0
26	BCR	t	102	40/40	0.97	0.07	1.59	21,29,48,53	0
30	GOL	V	205	6/6	0.98	0.09	1.57	26,34,37,43	0
28	SQD	a	424	54/54	0.80	0.26	1.57	63,83,134,198	0
30	GOL	B	626	6/6	0.93	0.12	1.54	34,41,49,61	0
24	CLA	B	602	65/65	0.95	0.10	1.50	27,39,92,115	0
32	LHG	d	409	49/49	0.99	0.08	1.49	27,37,48,52	0
29	LMG	c	520	51/55	0.85	0.22	1.48	47,76,100,124	0
32	LHG	B	632	49/49	0.98	0.08	1.46	20,30,52,61	0
32	LHG	d	411	49/49	0.98	0.09	1.38	26,31,79,84	0
26	BCR	C	525	40/40	0.96	0.10	1.36	26,33,39,41	0
36	EDO	d	417	4/4	0.97	0.09	1.34	46,49,52,58	0
40	DGD	H	103	62/66	0.97	0.08	1.32	21,31,45,54	0
35	P6G	D	416	19/19	0.97	0.07	1.29	38,60,84,87	0
24	CLA	a	410	65/65	0.97	0.09	1.29	20,25,98,113	0
34	PGE	o	308	10/10	0.87	0.22	1.28	48,87,100,104	0
29	LMG	B	621	51/55	0.97	0.07	1.27	27,39,54,88	0
32	LHG	E	101	42/49	0.90	0.18	1.26	54,80,100,127	0
32	LHG	e	101	42/49	0.82	0.27	1.25	60,105,123,171	0
31	LMT	b	622	35/35	0.81	0.22	1.23	49,76,124,132	0
32	LHG	D	410	49/49	0.99	0.08	1.21	21,27,41,48	0
29	LMG	J	101	47/55	0.97	0.07	1.19	23,29,74,83	0
31	LMT	Y	101	35/35	0.38	0.39	1.18	61,118,170,188	0
26	BCR	C	514	40/40	0.94	0.10	1.14	31,41,50,57	0
36	EDO	D	419	4/4	0.76	0.33	1.14	66,70,78,97	0
26	BCR	T	102	40/40	0.97	0.07	1.14	20,29,45,60	0
39	1PE	x	104	16/16	0.76	0.36	1.12	85,105,130,136	0
33	PG4	a	420	13/13	0.84	0.18	1.08	79,94,105,106	0
32	LHG	d	410	49/49	0.98	0.08	1.07	21,27,42,51	0
25	PHO	d	401	64/64	0.98	0.07	1.03	20,25,31,41	0
30	GOL	b	626	6/6	0.91	0.10	1.00	42,46,50,54	0
24	CLA	A	606	65/65	0.99	0.08	0.97	14,18,27,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	PG4	I	104	13/13	0.87	0.15	0.97	65,73,90,93	0
28	SQD	x	101	54/54	0.89	0.20	0.97	62,84,132,147	0
30	GOL	o	305	6/6	0.95	0.08	0.97	51,56,61,62	0
30	GOL	b	625	6/6	0.98	0.07	0.96	34,39,44,54	0
24	CLA	C	510	65/65	0.97	0.07	0.95	22,29,41,48	0
40	DGD	C	517	56/66	0.98	0.07	0.95	21,31,74,88	0
26	BCR	b	619	40/40	0.97	0.07	0.93	21,28,47,57	0
26	BCR	b	620	40/40	0.97	0.07	0.91	24,32,45,48	0
40	DGD	c	516	62/66	0.97	0.08	0.88	23,35,77,86	0
24	CLA	d	404	65/65	0.99	0.07	0.87	17,21,37,43	0
26	BCR	c	514	40/40	0.93	0.12	0.86	39,51,58,60	0
31	LMT	I	101	35/35	0.91	0.15	0.85	57,83,111,113	0
26	BCR	d	406	40/40	0.94	0.08	0.85	28,36,70,82	0
26	BCR	K	101	40/40	0.97	0.08	0.85	27,36,45,47	0
26	BCR	D	406	40/40	0.95	0.07	0.81	23,28,60,65	0
24	CLA	B	605	65/65	0.98	0.06	0.80	17,21,55,58	0
26	BCR	B	618	40/40	0.98	0.07	0.78	21,25,33,34	0
26	BCR	C	515	40/40	0.97	0.09	0.75	28,33,52,59	0
26	BCR	k	101	40/40	0.96	0.08	0.75	34,40,51,54	0
32	LHG	D	409	49/49	0.98	0.07	0.73	25,35,45,55	0
26	BCR	B	619	40/40	0.97	0.07	0.72	20,26,50,62	0
24	CLA	d	405	65/65	0.97	0.08	0.72	25,33,91,101	0
34	PGE	a	422	10/10	0.93	0.15	0.71	72,75,85,92	0
24	CLA	B	608	65/65	0.98	0.06	0.70	16,20,32,38	0
24	CLA	a	407	65/65	0.98	0.07	0.70	17,20,27,41	0
24	CLA	c	512	65/65	0.95	0.09	0.68	30,44,74,79	0
29	LMG	j	101	47/55	0.97	0.09	0.68	26,35,80,91	0
24	CLA	C	512	65/65	0.96	0.08	0.67	31,39,74,85	0
29	LMG	c	519	51/55	0.94	0.12	0.67	34,67,104,112	0
24	CLA	C	513	65/65	0.93	0.11	0.67	33,44,73,92	0
38	HTG	B	623	19/19	0.96	0.09	0.66	28,40,74,88	0
24	CLA	c	509	65/65	0.99	0.07	0.61	25,33,52,53	0
38	HTG	B	630	19/19	0.93	0.10	0.59	38,50,78,82	0
31	LMT	B	622	35/35	0.86	0.16	0.58	46,73,107,123	0
38	HTG	b	623	19/19	0.97	0.09	0.57	26,42,77,81	0
27	PL9	D	407	55/55	0.98	0.07	0.55	17,22,33,48	0
30	GOL	C	524	6/6	0.99	0.07	0.55	21,22,24,26	0
26	BCR	c	527	40/40	0.97	0.09	0.54	34,42,53,59	0
30	GOL	b	630	6/6	0.97	0.08	0.52	30,39,52,53	0
24	CLA	c	511	65/65	0.97	0.08	0.50	28,36,47,52	0
24	CLA	c	510	65/65	0.98	0.06	0.50	26,32,41,48	0
24	CLA	c	513	65/65	0.94	0.10	0.48	37,51,89,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	GOL	c	526	6/6	0.98	0.07	0.48	24,28,29,32	0
30	GOL	F	101	6/6	0.96	0.11	0.48	43,48,50,54	0
27	PL9	d	407	55/55	0.98	0.07	0.46	19,24,31,39	0
24	CLA	b	605	65/65	0.98	0.06	0.45	17,23,53,59	0
29	LMG	C	519	51/55	0.96	0.10	0.44	29,59,104,117	0
24	CLA	b	608	65/65	0.98	0.06	0.42	17,22,31,37	0
30	GOL	B	627	6/6	0.96	0.08	0.42	35,44,48,48	0
41	HEM	e	107	43/43	0.97	0.10	0.41	40,47,74,103	0
26	BCR	B	620	40/40	0.98	0.06	0.40	22,31,46,50	0
40	DGD	C	516	62/66	0.98	0.07	0.40	20,31,90,104	0
38	HTG	b	631	19/19	0.93	0.11	0.39	41,48,77,98	0
32	LHG	l	101	49/49	0.99	0.07	0.37	23,30,49,62	0
25	PHO	a	409	64/64	0.98	0.07	0.35	17,21,26,32	0
40	DGD	c	517	57/66	0.97	0.07	0.34	27,34,75,108	0
41	HEM	v	202	43/43	0.98	0.08	0.33	26,31,34,38	0
26	BCR	b	618	40/40	0.98	0.07	0.33	19,26,33,37	0
24	CLA	D	403	65/65	0.99	0.06	0.33	14,18,28,44	0
24	CLA	B	610	65/65	0.98	0.07	0.32	22,27,33,37	0
24	CLA	C	506	65/65	0.97	0.08	0.32	28,39,97,106	0
38	HTG	b	624	19/19	0.77	0.23	0.32	54,91,117,133	0
24	CLA	b	610	65/65	0.98	0.07	0.30	23,30,35,44	0
24	CLA	A	609	65/65	0.98	0.07	0.30	19,24,109,130	0
26	BCR	A	610	40/40	0.98	0.07	0.28	20,25,32,35	0
24	CLA	B	607	55/65	0.98	0.06	0.27	19,25,33,49	0
28	SQD	A	612	54/54	0.97	0.07	0.27	31,55,78,87	0
25	PHO	D	401	64/64	0.98	0.06	0.26	17,23,31,41	0
24	CLA	b	607	55/65	0.98	0.07	0.24	22,27,36,49	0
30	GOL	b	627	6/6	0.97	0.07	0.23	40,47,52,54	0
24	CLA	c	506	65/65	0.96	0.08	0.22	26,37,83,95	0
24	CLA	b	617	60/65	0.95	0.10	0.20	26,31,82,92	0
30	GOL	O	302	6/6	0.88	0.12	0.20	51,55,67,70	0
24	CLA	a	408	60/65	0.98	0.07	0.18	18,25,73,85	0
24	CLA	C	504	60/65	0.98	0.06	0.17	20,26,70,81	0
24	CLA	C	508	60/65	0.98	0.07	0.16	23,29,51,61	0
30	GOL	B	628	6/6	0.99	0.07	0.16	34,40,48,49	0
25	PHO	A	608	64/64	0.98	0.06	0.13	17,19,26,26	0
24	CLA	c	508	60/65	0.98	0.06	0.13	23,29,52,62	0
24	CLA	c	503	65/65	0.97	0.07	0.13	26,35,42,52	0
31	LMT	M	101	35/35	0.86	0.14	0.11	34,51,70,73	0
34	PGE	Y	102	10/10	0.81	0.17	0.10	61,84,103,104	0
24	CLA	b	603	65/65	0.98	0.07	0.07	21,28,39,43	0
24	CLA	B	606	65/65	0.98	0.07	0.07	18,22,34,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	CLA	c	502	65/65	0.99	0.07	0.05	24,30,41,50	0
24	CLA	b	613	65/65	0.98	0.07	0.03	20,25,32,41	0
30	GOL	a	415	6/6	0.97	0.07	0.03	29,39,45,45	0
24	CLA	b	606	65/65	0.98	0.06	0.02	20,25,33,39	0
24	CLA	d	403	65/65	0.99	0.05	0.02	17,20,29,38	0
30	GOL	B	629	6/6	0.97	0.08	0.02	31,39,60,64	0
26	BCR	c	515	40/40	0.97	0.08	0.01	26,35,47,55	0
30	GOL	o	304	6/6	0.97	0.07	0.01	45,53,55,62	0
24	CLA	C	502	65/65	0.98	0.06	0.00	21,27,37,54	0
28	SQD	a	413	54/54	0.98	0.07	0.00	33,54,92,96	0
24	CLA	C	511	65/65	0.97	0.08	-0.01	26,33,40,45	0
24	CLA	C	503	65/65	0.98	0.06	-0.01	26,30,38,43	0
24	CLA	A	607	60/65	0.98	0.06	-0.06	17,20,66,78	0
31	LMT	m	102	35/35	0.90	0.12	-0.06	28,50,66,82	0
24	CLA	B	603	65/65	0.98	0.06	-0.08	21,26,33,38	0
24	CLA	c	504	60/65	0.97	0.06	-0.08	25,31,67,75	0
24	CLA	C	505	65/65	0.98	0.06	-0.11	23,29,47,52	0
24	CLA	D	405	65/65	0.98	0.06	-0.12	22,29,91,98	0
24	CLA	D	404	65/65	0.98	0.06	-0.13	13,18,35,40	0
30	GOL	v	204	6/6	0.99	0.06	-0.14	30,36,41,50	0
24	CLA	b	614	65/65	0.98	0.06	-0.14	19,23,48,54	0
40	DGD	c	518	62/66	0.98	0.06	-0.15	25,36,65,81	0
30	GOL	V	201	6/6	0.97	0.06	-0.16	28,30,35,39	0
41	HEM	V	203	43/43	0.99	0.06	-0.20	20,24,27,29	0
26	BCR	a	411	40/40	0.97	0.06	-0.22	20,25,31,32	0
24	CLA	B	613	65/65	0.98	0.06	-0.22	17,23,30,39	0
30	GOL	b	628	6/6	0.98	0.06	-0.22	32,34,35,44	0
41	HEM	E	113	43/43	0.98	0.07	-0.24	35,42,61,68	0
24	CLA	c	505	65/65	0.98	0.06	-0.25	25,29,44,50	0
24	CLA	b	612	65/65	0.99	0.06	-0.26	18,24,37,42	0
30	GOL	v	206	6/6	0.95	0.09	-0.27	50,54,66,75	0
26	BCR	H	102	40/40	0.96	0.08	-0.33	23,33,52,55	0
24	CLA	B	609	65/65	0.99	0.06	-0.34	19,24,33,40	0
24	CLA	c	507	65/65	0.98	0.07	-0.37	28,34,50,59	0
24	CLA	B	617	60/65	0.97	0.07	-0.37	21,27,90,107	0
24	CLA	B	614	65/65	0.98	0.06	-0.39	17,21,48,64	0
26	BCR	h	103	40/40	0.97	0.06	-0.40	25,35,50,53	0
24	CLA	C	501	65/65	0.98	0.06	-0.46	25,30,48,57	0
24	CLA	c	501	65/65	0.98	0.06	-0.51	27,35,49,53	0
24	CLA	B	611	65/65	0.98	0.06	-0.54	20,24,38,51	0
24	CLA	b	604	65/65	0.99	0.05	-0.54	22,28,38,45	0
24	CLA	C	507	65/65	0.98	0.06	-0.55	27,33,48,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	GOL	V	208	6/6	0.97	0.07	-0.57	65,70,82,83	0
24	CLA	B	604	65/65	0.99	0.05	-0.64	19,23,34,41	0
37	CA	O	301	1/1	0.98	0.08	-0.70	53,53,53,53	0
24	CLA	b	615	65/65	0.98	0.06	-0.71	18,26,94,117	0
37	CA	c	524	1/1	1.00	0.08	-0.72	45,45,45,45	0
24	CLA	B	616	65/65	0.98	0.06	-0.75	21,27,48,56	0
37	CA	o	302	1/1	0.98	0.08	-0.76	55,55,55,55	0
24	CLA	b	609	65/65	0.99	0.05	-0.77	22,27,37,44	0
24	CLA	B	615	55/65	0.98	0.05	-0.78	17,23,55,82	0
23	BCT	A	605	4/4	0.98	0.06	-0.81	27,31,35,52	0
24	CLA	b	611	65/65	0.98	0.05	-0.82	23,28,38,44	0
24	CLA	B	612	65/65	0.99	0.05	-0.82	16,21,35,39	0
23	BCT	a	406	4/4	0.98	0.05	-0.83	27,28,31,49	0
42	MG	j	102	1/1	0.99	0.05	-0.93	35,35,35,35	0
24	CLA	b	616	65/65	0.98	0.05	-1.01	22,29,47,56	0
42	MG	J	102	1/1	0.99	0.04	-1.33	27,27,27,27	0
22	CL	A	604	1/1	1.00	0.03	-1.57	21,21,21,21	0
21	FE2	a	403	1/1	1.00	0.02	-2.11	25,25,25,25	0
21	FE2	A	602	1/1	1.00	0.02	-2.54	25,25,25,25	0
22	CL	a	405	1/1	1.00	0.02	-2.78	25,25,25,25	0
20	OEX	A	601	10/10	1.00	0.02	-2.86	20,21,24,26	0
20	OEX	a	402	10/10	1.00	0.02	-2.92	23,24,26,27	0
22	CL	A	603	1/1	1.00	0.01	-2.98	23,23,23,23	0
22	CL	a	404	1/1	1.00	0.02	-3.21	28,28,28,28	0
31	LMT	C	533	35/35	0.52	0.56	-	72,121,170,191	0
38	HTG	C	531	19/19	0.73	0.44	-	72,109,139,142	0
34	PGE	E	105	10/10	0.68	0.60	-	90,96,116,118	0
34	PGE	E	107	10/10	0.54	0.59	-	73,106,142,143	0
34	PGE	H	108	10/10	0.83	0.29	-	66,86,129,136	0
38	HTG	C	532	19/19	0.72	0.32	-	57,85,128,156	0
33	PG4	I	103	13/13	0.82	0.23	-	73,97,121,129	0
33	PG4	h	106	13/13	0.93	0.22	-	67,76,106,108	0
34	PGE	O	310	10/10	0.86	0.58	-	58,81,122,137	0
34	PGE	J	108	10/10	0.87	0.29	-	80,98,116,120	0
30	GOL	f	104	6/6	0.84	0.31	-	94,115,135,150	0
34	PGE	h	109	10/10	0.79	0.48	-	84,97,111,113	0
33	PG4	B	638	13/13	0.80	0.35	-	66,84,114,130	0
34	PGE	t	104	10/10	0.93	0.09	-	60,79,99,100	0
33	PG4	c	535	13/13	0.78	0.35	-	69,89,109,115	0
35	P6G	I	106	19/19	0.74	0.26	-	56,81,119,121	0
33	PG4	B	643	13/13	0.74	0.45	-	75,92,114,118	0
34	PGE	j	105	10/10	0.87	0.22	-	73,109,124,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	GOL	d	413	6/6	0.90	0.17	-	74,88,114,116	0
34	PGE	B	650	10/10	0.68	0.50	-	88,109,126,128	0
35	P6G	b	648	19/19	0.93	0.11	-	59,66,80,84	0
33	PG4	B	641	13/13	0.81	0.33	-	74,97,107,115	0
36	EDO	C	542	4/4	0.79	0.48	-	77,84,88,96	0
30	GOL	e	102	6/6	0.78	0.35	-	79,91,112,117	0
34	PGE	b	645	10/10	0.78	0.44	-	106,110,126,134	0
35	P6G	C	541	19/19	0.69	0.49	-	79,103,127,142	0
36	EDO	i	108	4/4	0.95	0.21	-	70,71,76,87	0
33	PG4	C	537	13/13	0.86	0.23	-	67,76,92,108	0
36	EDO	J	109	4/4	0.95	0.10	-	78,79,85,96	0
39	1PE	B	653	16/16	0.41	0.61	-	103,121,137,148	0
34	PGE	b	641	10/10	0.85	0.22	-	99,104,114,125	0
33	PG4	D	414	13/13	0.87	0.34	-	86,95,105,110	0
38	HTG	C	521	19/19	0.95	0.13	-	53,65,84,85	0
34	PGE	B	644	10/10	0.94	0.09	-	58,71,117,137	0
34	PGE	J	106	10/10	0.60	0.40	-	85,121,129,138	0
33	PG4	C	538	13/13	0.75	0.34	-	65,93,115,123	0
34	PGE	h	110	10/10	0.64	0.27	-	71,99,111,117	0
33	PG4	b	637	13/13	0.71	0.52	-	74,97,124,130	0
37	CA	b	601	1/1	0.98	0.19	-	72,72,72,72	0
36	EDO	o	311	4/4	0.76	0.35	-	81,83,83,86	0
38	HTG	C	530	19/19	0.70	0.48	-	98,124,143,150	0
33	PG4	E	103	13/13	0.74	0.24	-	59,76,89,105	0
30	GOL	O	307	6/6	0.35	0.78	-	116,117,120,123	0
30	GOL	u	201	6/6	0.90	0.24	-	43,70,71,77	0
36	EDO	B	658	4/4	0.95	0.26	-	82,84,89,110	0
34	PGE	B	647	10/10	0.90	0.31	-	78,92,122,122	0
33	PG4	b	634	13/13	0.71	0.29	-	78,90,111,123	0
34	PGE	b	639	10/10	0.76	0.45	-	79,97,111,119	0
36	EDO	B	657	4/4	0.77	0.34	-	93,95,100,102	0
42	MG	F	103	1/1	0.98	0.10	-	32,32,32,32	0
33	PG4	l	103	13/13	0.95	0.08	-	48,64,71,74	0
39	1PE	j	107	16/16	0.66	0.30	-	74,106,155,159	0
22	CL	V	202	1/1	0.97	0.06	-	68,68,68,68	0
34	PGE	b	646	10/10	0.55	0.45	-	70,102,120,121	0
33	PG4	B	636	13/13	0.67	0.35	-	71,98,116,121	0
37	CA	B	601	1/1	0.98	0.21	-	82,82,82,82	0
36	EDO	a	425	4/4	0.92	0.24	-	74,78,96,120	0
34	PGE	a	423	10/10	0.86	0.26	-	78,91,107,107	0
33	PG4	i	101	13/13	0.86	0.17	-	71,84,95,98	0
36	EDO	E	111	4/4	0.63	0.24	-	66,83,90,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	EDO	I	107	4/4	0.86	0.16	-	84,89,91,96	0
35	P6G	c	541	19/19	0.78	0.33	-	43,61,68,72	19
30	GOL	o	303	6/6	0.70	0.47	-	79,96,110,126	0
30	GOL	y	101	6/6	0.70	0.30	-	82,90,98,101	0
34	PGE	b	644	10/10	0.70	0.47	-	83,100,113,125	0
34	PGE	I	105	10/10	0.78	0.20	-	60,83,95,99	0
34	PGE	H	110	10/10	0.77	0.53	-	91,103,116,118	0
34	PGE	H	109	10/10	0.77	0.38	-	84,95,102,105	0
33	PG4	H	105	13/13	0.84	0.25	-	72,87,126,147	0
33	PG4	e	103	13/13	0.54	0.41	-	72,107,125,136	0
34	PGE	c	536	10/10	0.54	0.58	-	87,105,124,125	0
30	GOL	C	527	6/6	0.81	0.49	-	96,108,112,135	0
34	PGE	b	640	10/10	0.90	0.21	-	61,88,103,118	0
30	GOL	T	103	6/6	0.93	0.14	-	62,79,91,111	0
34	PGE	E	106	10/10	0.69	0.35	-	85,95,111,116	0
34	PGE	A	620	7/10	0.85	0.11	-	68,77,83,87	0
34	PGE	i	106	10/10	0.53	0.52	-	78,95,100,103	0
33	PG4	V	213	13/13	0.82	0.48	-	68,80,103,112	0
34	PGE	h	108	10/10	0.73	0.30	-	70,75,101,105	0
36	EDO	H	112	4/4	0.86	0.27	-	70,85,94,95	0
34	PGE	E	108	10/10	0.53	0.41	-	52,65,68,73	10
43	2PE	i	107	25/28	0.90	0.14	-	44,66,104,122	0
34	PGE	H	111	10/10	0.74	0.36	-	82,100,121,127	0
38	HTG	B	624	19/19	0.74	0.28	-	47,103,125,143	0
33	PG4	H	106	13/13	0.75	0.31	-	38,53,67,74	13
34	PGE	b	647	10/10	0.71	0.59	-	77,97,109,109	0
34	PGE	x	103	10/10	0.86	0.57	-	81,98,110,112	0
36	EDO	V	218	4/4	0.70	0.46	-	87,88,88,96	0
30	GOL	m	103	6/6	0.94	0.15	-	47,69,88,116	0
33	PG4	B	640	13/13	0.72	0.22	-	66,86,95,99	0
22	CL	v	201	1/1	0.98	0.07	-	72,72,72,72	0
36	EDO	c	542	4/4	0.75	0.68	-	88,91,102,107	0
34	PGE	h	107	10/10	0.90	0.17	-	67,78,92,95	0
34	PGE	A	621	10/10	0.83	0.20	-	66,116,120,129	0
33	PG4	C	534	13/13	0.55	0.55	-	81,103,119,119	0
34	PGE	c	538	10/10	0.82	0.29	-	68,102,115,129	0
33	PG4	X	103	13/13	0.66	0.38	-	78,99,111,115	0
33	PG4	i	103	13/13	0.80	0.37	-	74,85,98,105	0
38	HTG	c	522	19/19	0.91	0.23	-	60,74,96,106	0
33	PG4	d	414	13/13	0.85	0.26	-	65,79,85,87	0
30	GOL	v	205	6/6	0.54	0.69	-	102,122,135,152	0
34	PGE	b	642	10/10	0.95	0.09	-	51,65,87,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	EDO	e	106	4/4	0.82	0.11	-	72,76,79,89	0
36	EDO	o	310	4/4	0.85	0.32	-	60,65,77,90	0
30	GOL	D	412	6/6	0.94	0.12	-	55,80,95,102	0
34	PGE	c	537	10/10	0.83	0.28	-	96,106,120,123	0
42	MG	f	102	1/1	0.99	0.07	-	45,45,45,45	0
35	P6G	b	649	19/19	0.80	0.26	-	71,103,125,128	0
36	EDO	A	625	4/4	0.76	0.16	-	70,71,80,80	0
36	EDO	B	655	4/4	0.95	0.31	-	45,50,57,88	0
38	HTG	B	631	19/19	0.78	0.21	-	46,90,129,147	0
30	GOL	B	633	6/6	0.87	0.16	-	69,71,84,97	0
34	PGE	J	107	10/10	0.68	0.26	-	87,137,168,170	0
34	PGE	f	105	10/10	0.42	0.54	-	91,98,114,127	0
38	HTG	c	530	19/19	0.68	0.31	-	66,104,128,145	0
33	PG4	i	104	13/13	0.84	0.15	-	56,71,90,91	0
39	1PE	L	101	16/16	0.92	0.12	-	56,72,99,100	0
35	P6G	B	651	19/19	0.95	0.07	-	49,63,77,81	0
34	PGE	D	415	10/10	0.62	0.61	-	86,105,110,122	0
33	PG4	H	104	13/13	0.83	0.38	-	83,98,117,119	0
37	CA	h	102	1/1	0.93	0.12	-	97,97,97,97	0
35	P6G	D	418	19/19	0.59	0.39	-	68,99,126,131	0
34	PGE	o	307	10/10	0.62	0.55	-	90,112,130,142	0
34	PGE	B	646	10/10	0.70	0.45	-	83,95,114,119	0
33	PG4	b	635	13/13	0.87	0.15	-	58,76,103,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.