



Full wwPDB X-ray Structure Validation Report

Aug 26, 2014 – 03:11 PM EDT

PDB ID : 3WU2
Title : Crystal structure analysis of Photosystem II complex
Authors : Umena, Y.; Kawakami, K.; Shen, J.R.; Kamiya, N.
Deposited on : 2014-04-21
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

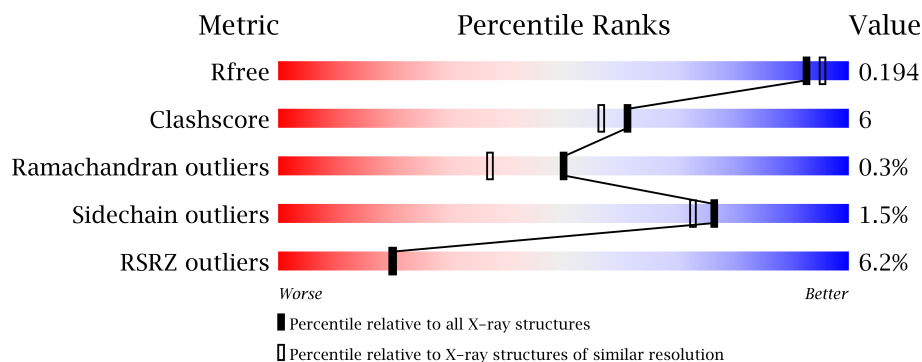
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	504	
2	b	504	
3	C	455	
3	c	455	
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	

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Mol	Chain	Length	Quality of chain
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	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
23	CLA	B	602	-	X
23	CLA	b	604	-	X
26	SQD	A	418	-	X
26	SQD	B	621	-	X
26	SQD	D	407	-	X
26	SQD	L	103	-	X
26	SQD	a	401	-	X
27	LMG	A	413	-	X
27	LMG	D	411	-	X
27	LMG	Z	101	-	X
27	LMG	c	921	-	X
28	PL9	A	414	-	X
28	PL9	a	419	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
29	UNL	A	416	-	X
29	UNL	A	417	-	X
29	UNL	A	420	-	X
29	UNL	B	628	-	X
29	UNL	B	629	-	X
29	UNL	B	632	-	X
29	UNL	C	523	-	X
29	UNL	D	412	-	X
29	UNL	D	413	-	X
29	UNL	E	102	-	X
29	UNL	E	103	-	X
29	UNL	H	103	-	X
29	UNL	I	101	-	X
29	UNL	I	102	-	X
29	UNL	J	104	-	X
29	UNL	M	103	-	X
29	UNL	T	102	-	X
29	UNL	X	101	-	X
29	UNL	a	403	-	X
29	UNL	a	420	-	X
29	UNL	a	421	-	X
29	UNL	b	628	-	X
29	UNL	b	630	-	X
29	UNL	b	631	-	X
29	UNL	c	925	-	X
29	UNL	c	926	-	X
29	UNL	d	411	-	X
29	UNL	e	800	-	X
29	UNL	i	101	-	X
29	UNL	i	102	-	X
29	UNL	i	103	-	X
29	UNL	i	104	-	X
29	UNL	j	102	-	X
29	UNL	t	103	-	X
29	UNL	x	101	-	X
29	UNL	z	102	-	X
30	LMT	A	419	-	X
30	LMT	F	102	-	X
30	LMT	J	102	-	X
30	LMT	M	101	-	X
30	LMT	b	625	-	X
30	LMT	c	922	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
30	LMT	t	102	-	X
31	GOL	A	422	-	X
31	GOL	A	423	-	X
31	GOL	B	633	-	X
31	GOL	B	636	-	X
31	GOL	B	638	-	X
31	GOL	C	524	-	X
31	GOL	C	526	-	X
31	GOL	D	415	-	X
31	GOL	L	104	-	X
31	GOL	V	204	-	X
31	GOL	V	205	-	X
31	GOL	a	422	-	X
31	GOL	a	423	-	X
31	GOL	a	424	-	X
31	GOL	b	632	-	X
31	GOL	b	633	-	X
31	GOL	c	927	-	X
31	GOL	c	928	-	X
31	GOL	c	930	-	X
31	GOL	f	104	-	X
31	GOL	l	102	-	X
33	HTG	B	626	-	X
33	HTG	B	631	-	X
33	HTG	C	522	-	X
33	HTG	D	414	-	X
33	HTG	U	201	-	X
33	HTG	V	202	-	X
33	HTG	b	601	-	X
33	HTG	b	602	-	X
33	HTG	b	626	-	X
33	HTG	c	923	-	X
33	HTG	c	924	-	X
33	HTG	d	401	-	X
33	HTG	u	201	-	X
34	DGD	C	518	-	X
34	DGD	D	406	-	X
34	DGD	d	406	-	X
36	LHG	D	410	-	X
36	LHG	a	417	-	X
36	LHG	d	407	-	X
39	MG	j	101	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
40	SO4	O	302	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54036 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2633	1729	429	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2625	1722	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4009	2633	668	695	13			
2	b	501	Total	C	N	O	S	0	11	0
			3964	2605	658	688	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	3	0
			3502	2291	588	610	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2315	593	615	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	SEE REMARK 999	UNP D0VWR7
C	20	SER	-	SEE REMARK 999	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	SEE REMARK 999	UNP D0VWR7
C	22	PHE	-	SEE REMARK 999	UNP D0VWR7
c	19	ASN	-	SEE REMARK 999	UNP D0VWR7
c	20	SER	-	SEE REMARK 999	UNP D0VWR7
c	21	ILE	-	SEE REMARK 999	UNP D0VWR7
c	22	PHE	-	SEE REMARK 999	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	341	Total	C	N	O	S	0	4	0
			2741	1817	449	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	0	0
			657	429	106	122				
5	e	79	Total	C	N	O		0	0	0
			639	419	103	117				

- 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
			274	187	45	41	1			
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	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			294	199	45	49	1			
8	i	38	Total	C	N	O	S	0	0	0
			311	210	48	52	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			271	182	40	48	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	1	0
			290	202	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	SEE REMARK 999	UNP P19054
K	39	TRP	VAL	SEE REMARK 999	UNP P19054
k	33	LEU	PHE	SEE REMARK 999	UNP P19054
k	39	TRP	VAL	SEE REMARK 999	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	0	1	0
			302	203	48	51			
11	l	37	Total	C	N	O	0	2	0
			300	204	45	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			261	176	37	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			271	184	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	SEE REMARK 999	UNP P12312
m	8	LEU	PHE	SEE REMARK 999	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	5	0
			1878	1177	314	382	5			
13	o	241	Total	C	N	O	S	0	5	0
			1855	1163	305	381	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

- 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	0	0
			770	489	129	152				
15	u	97	Total	C	N	O		0	1	0
			772	490	129	153				

- 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
			1066	677	180	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	130	32	31	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

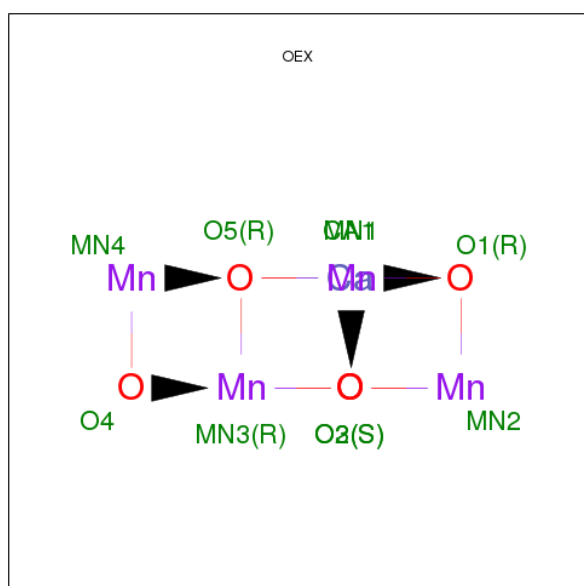
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O		0	1	0
			280	190	44	46				

- 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
			459	318	67	73	1			
19	z	60	Total	C	N	O	S	0	0	0
			431	301	64	65	1			

- 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		

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

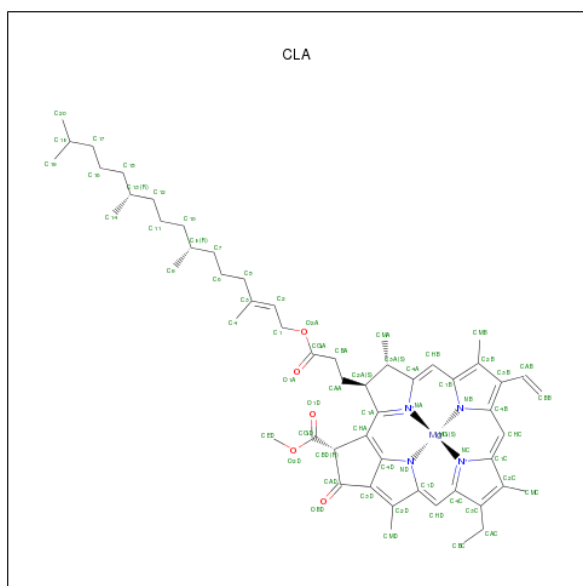
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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				

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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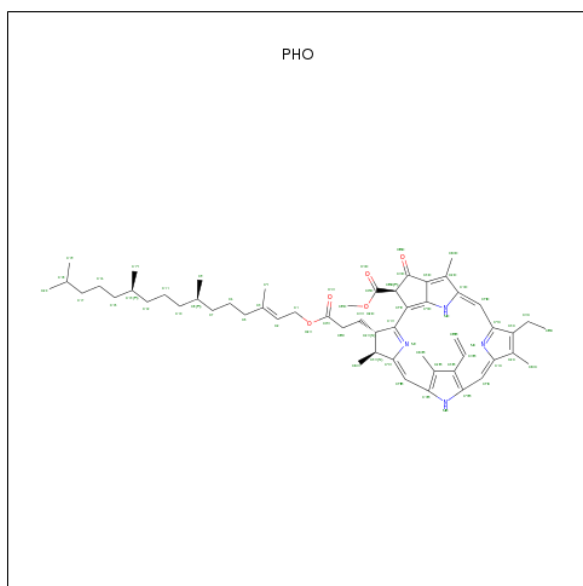
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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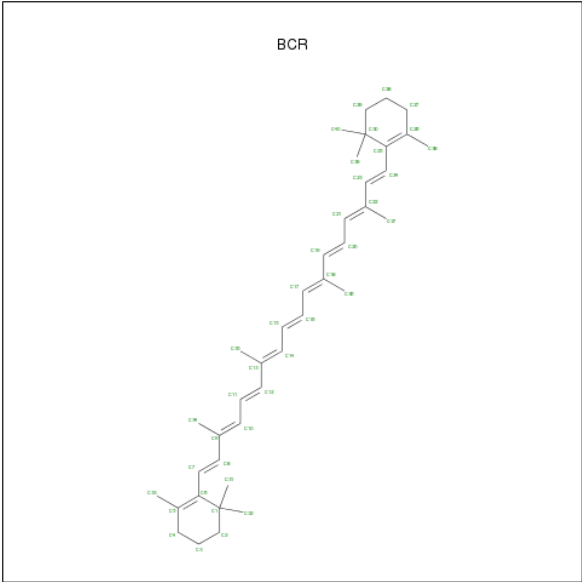
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



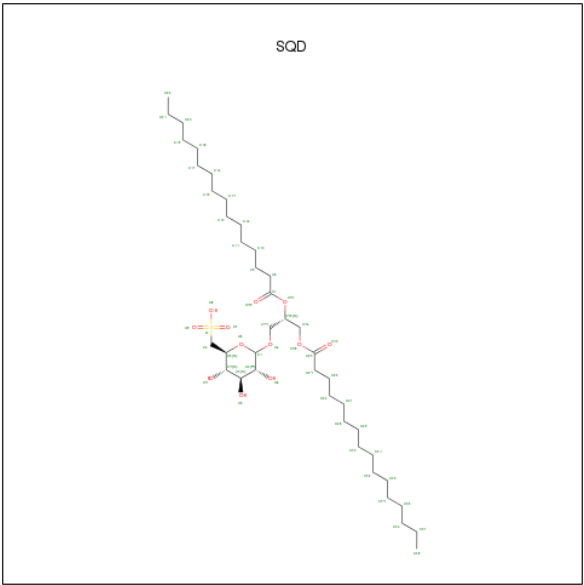
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	a	1	Total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

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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



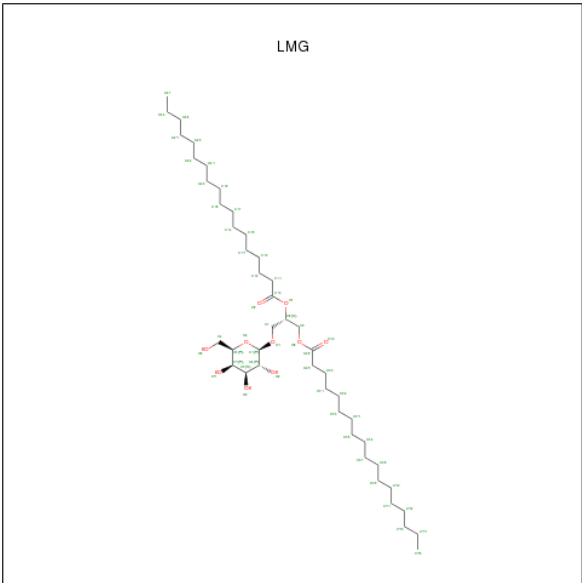
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			33	23	9	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



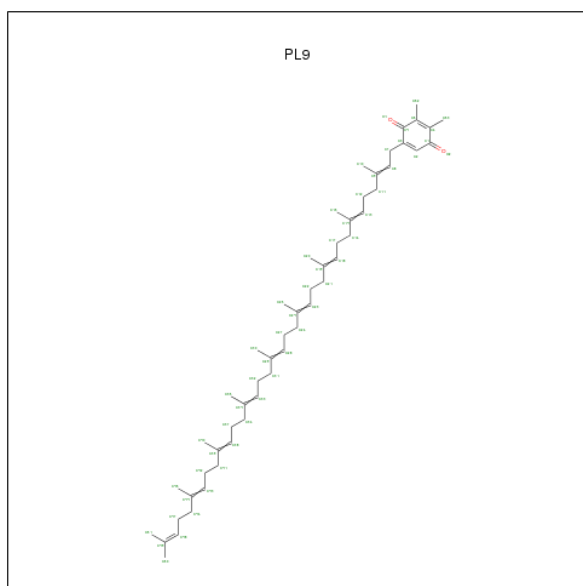
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	B	1	Total	C	O	0	0
			51	41	10		
27	C	1	Total	C	O	0	0
			51	41	10		
27	D	1	Total	C	O	0	0
			51	41	10		
27	Z	1	Total	C	O	0	0
			51	41	10		
27	a	1	Total	C	O	0	0
			51	41	10		
27	b	1	Total	C	O	0	0
			51	41	10		
27	c	1	Total	C	O	0	0
			51	41	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	0
			51	41	10		
27	d	1	Total	C	O	0	0
			51	41	10		

- Molecule 28 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
28	A	1	Total	C	O	0	0
			55	53	2		
28	D	1	Total	C	O	0	0
			55	53	2		
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

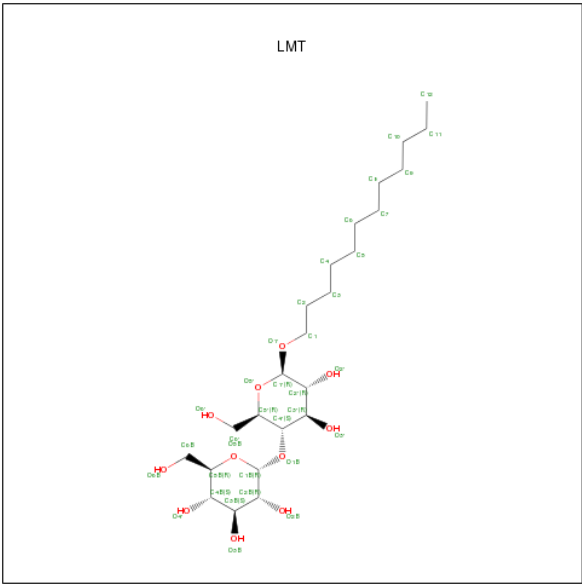
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	B	4	Total	C		0	0
			56	56			
29	c	2	Total	C	O	0	0
			40	35	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	t	1	Total C 16 16	0	0
29	X	1	Total C 16 16	0	0
29	J	2	Total C 26 26	0	0
29	E	2	Total C 27 27	0	0
29	b	4	Total C O 84 79 5	0	0
29	A	4	Total C O 69 64 5	0	0
29	x	1	Total C 16 16	0	0
29	M	1	Total C 16 16	0	0
29	j	2	Total C 28 28	0	0
29	D	2	Total C O 56 51 5	0	0
29	e	1	Total C 11 11	0	0
29	I	2	Total C 24 24	0	0
29	Z	1	Total C 16 16	0	0
29	a	3	Total C O 56 51 5	0	0
29	L	1	Total C 14 14	0	0
29	d	1	Total C 16 16	0	0
29	H	1	Total C 10 10	0	0
29	i	4	Total C 55 55	0	0
29	C	1	Total C O 34 29 5	0	0
29	z	1	Total C 16 16	0	0
29	T	1	Total C 13 13	0	0

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



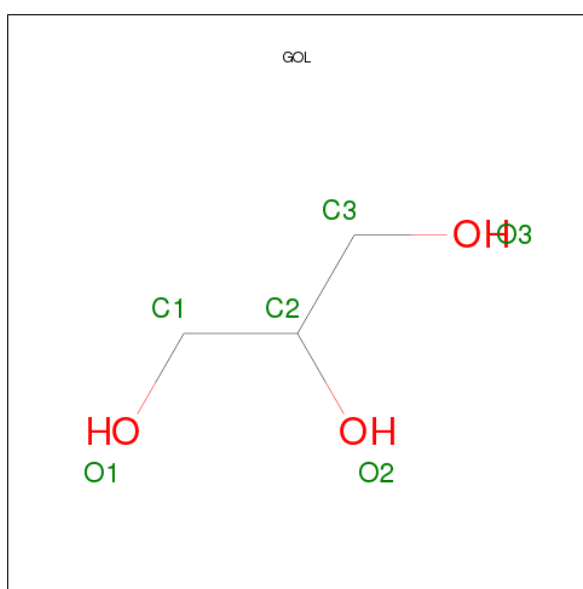
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	C	1	Total	C	O	0	0
			35	24	11		
30	F	1	Total	C	O	0	0
			35	24	11		
30	J	1	Total	C	O	0	0
			24	18	6		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	Z	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	b	1	Total	C	O	0	0
			24	18	6		
30	c	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	t	1	Total	C	O	0	0
			24	18	6		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 6	C 3	O 3	0	0
31	B	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	D	1	Total 6	C 3	O 3	0	0
31	L	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0

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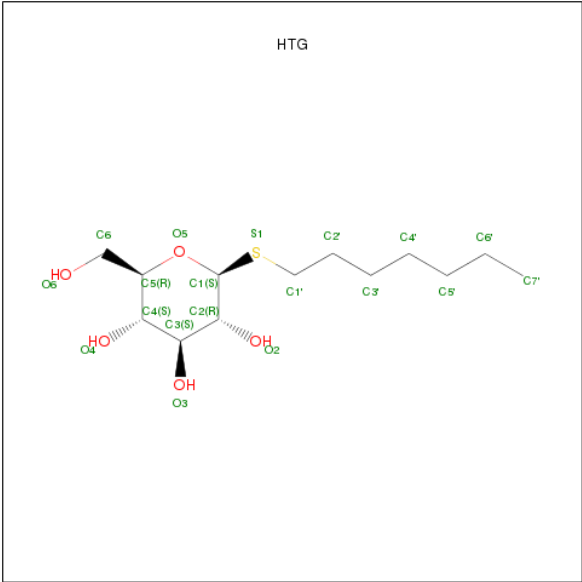
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 6 3 3	0	0
31	c	1	Total C O 6 3 3	0	0
31	f	1	Total C O 6 3 3	0	0
31	h	1	Total C O 6 3 3	0	0
31	l	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total Ca 1 1	0	0
32	c	1	Total Ca 1 1	0	0
32	F	1	Total Ca 1 1	0	0
32	o	1	Total Ca 1 1	0	0
32	O	1	Total Ca 1 1	0	0
32	b	1	Total Ca 1 1	0	0
32	f	1	Total Ca 1 1	0	0

- Molecule 33 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



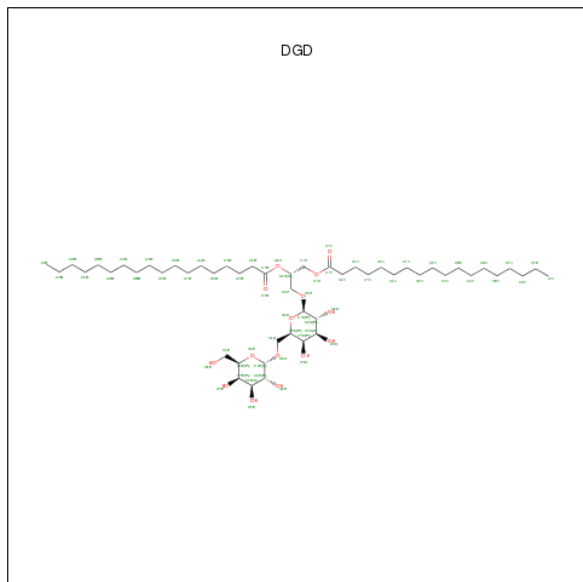
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	C	1	Total C O S 19 13 5 1	0	0
33	C	1	Total C O S 19 13 5 1	0	0
33	D	1	Total C O S 19 13 5 1	0	0
33	O	1	Total C O S 19 13 5 1	0	0
33	U	1	Total C S 9 8 1	0	0
33	V	1	Total C O S 13 7 5 1	0	0
33	b	1	Total C O S 19 13 5 1	0	0
33	b	1	Total C O S 19 13 5 1	0	0
33	b	1	Total C O S 19 13 5 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	b	1	Total	C	O	S	0	0
			19	13	5	1		
33	c	1	Total	C	O	S	0	0
			19	13	5	1		
33	c	1	Total	C	O	S	0	0
			19	13	5	1		
33	d	1	Total	C	O	S	0	0
			19	13	5	1		
33	u	1	Total	C	O	S	0	0
			14	10	3	1		

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



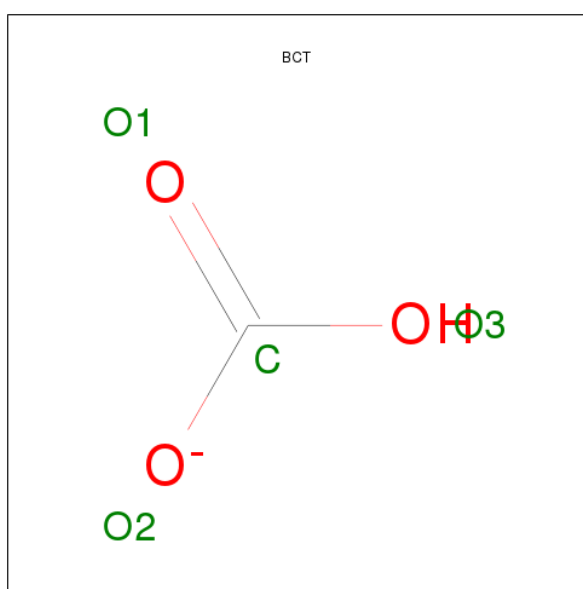
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	D	1	Total	C	O		0	0
			53	42	11			
34	H	1	Total	C	O		0	0
			62	47	15			
34	c	1	Total	C	O		0	0
			62	47	15			

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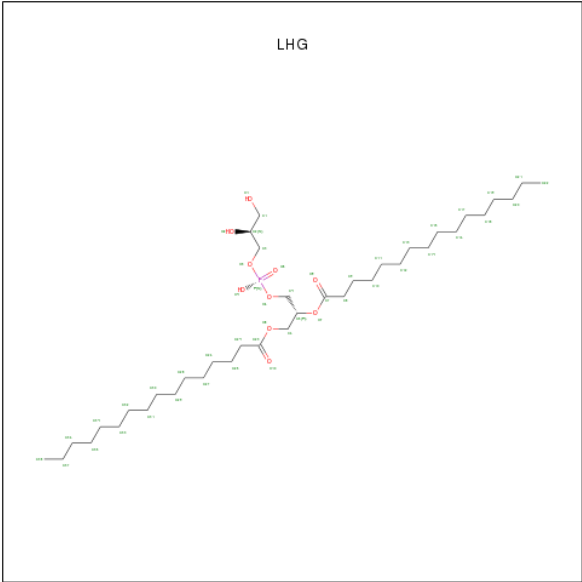
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		
34	d	1	Total	C	O	0	0
			50	41	9		
34	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 35 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



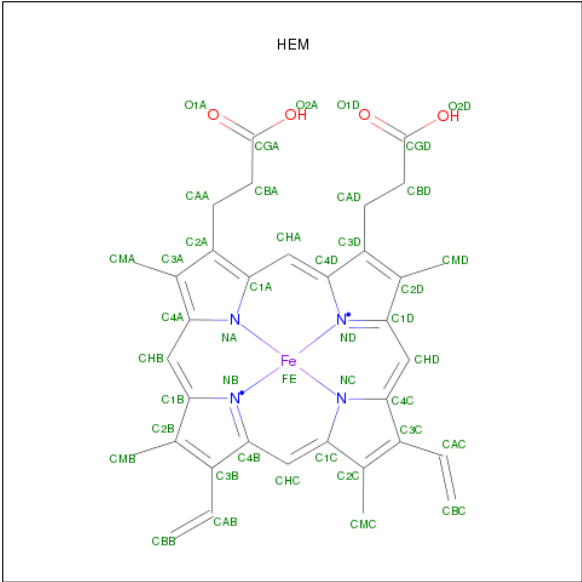
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	D	1	Total	C	O	0	0
			4	1	3		
35	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



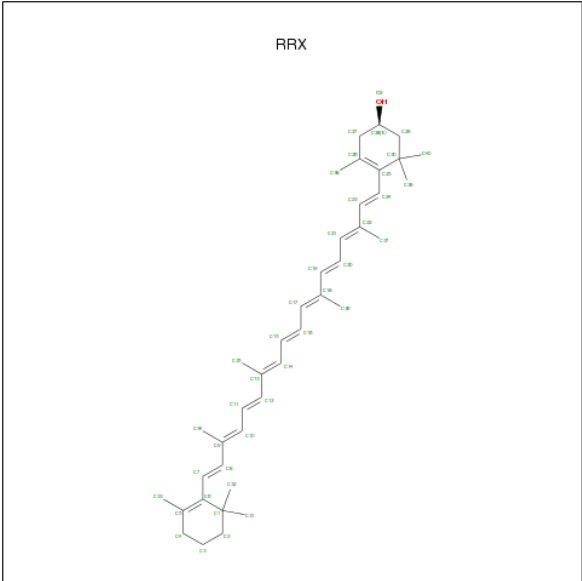
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			46	35	10	1		
36	E	1	Total	C	O	P	0	0
			49	38	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	a	1	Total	C	O	P	0	0
			40	29	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
37	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
37	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
37	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 38 is (3R)-BETA,BETA-CAROTEN-3-OL (three-letter code: RRX) (formula: $C_{40}H_{56}O$).

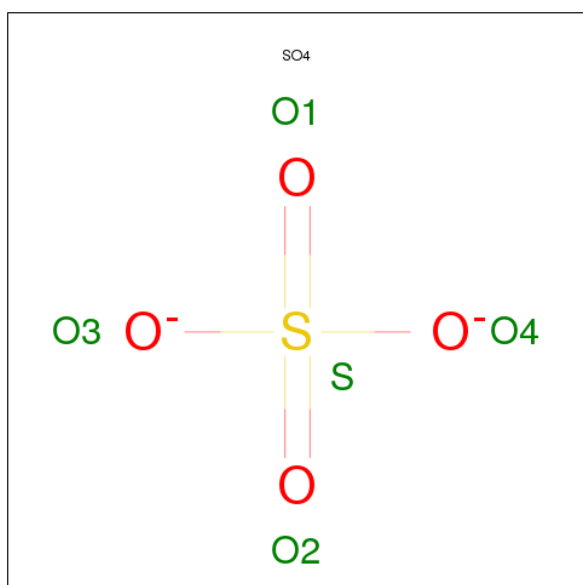


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	h	1	Total	C	O	0	0
			41	40	1		

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

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

- Molecule 40 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	168	Total	O	0	2
			170	170		
41	B	311	Total	O	0	8
			319	319		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	C	253	Total 263	O 263	0	10
41	D	156	Total 161	O 161	0	5
41	E	32	Total 35	O 35	0	3
41	F	12	Total 12	O 12	0	0
41	H	50	Total 52	O 52	0	2
41	I	8	Total 8	O 8	0	0
41	J	9	Total 9	O 9	0	0
41	K	8	Total 8	O 8	0	0
41	L	23	Total 24	O 24	0	1
41	M	15	Total 16	O 16	0	1
41	O	193	Total 202	O 202	0	9
41	T	10	Total 10	O 10	0	0
41	U	98	Total 100	O 100	0	2
41	V	140	Total 144	O 144	0	4
41	Y	6	Total 6	O 6	0	0
41	X	13	Total 14	O 14	0	1
41	Z	1	Total 1	O 1	0	0
41	a	153	Total 155	O 155	0	2
41	b	295	Total 306	O 306	0	11
41	c	238	Total 245	O 245	0	7
41	d	156	Total 160	O 160	0	4

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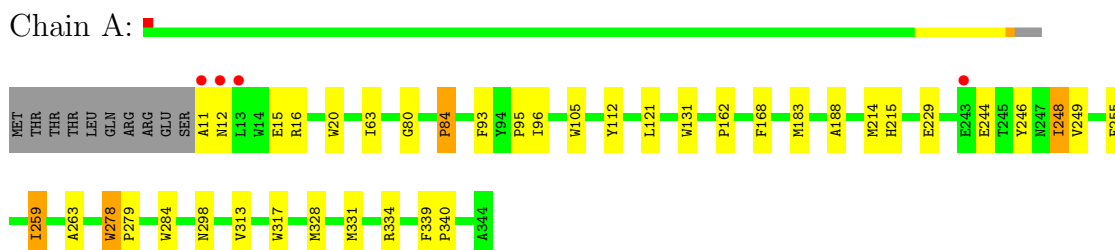
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	e	22	Total 22	O 22	0	0
41	f	13	Total 14	O 14	0	1
41	h	48	Total 53	O 53	0	5
41	i	13	Total 14	O 14	0	1
41	j	9	Total 9	O 9	0	0
41	k	5	Total 5	O 5	0	0
41	l	17	Total 18	O 18	0	1
41	m	15	Total 16	O 16	0	1
41	o	167	Total 175	O 175	0	8
41	t	12	Total 12	O 12	0	0
41	u	102	Total 106	O 106	0	4
41	v	98	Total 104	O 104	0	6
41	y	7	Total 7	O 7	0	0
41	x	6	Total 6	O 6	0	0
41	z	2	Total 2	O 2	0	0

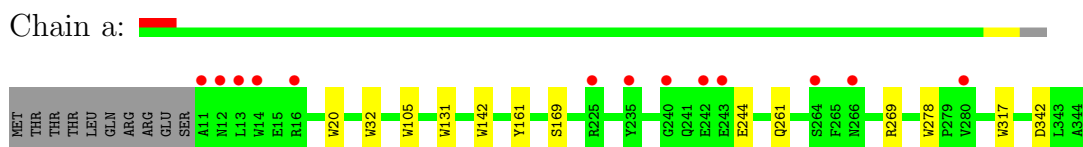
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

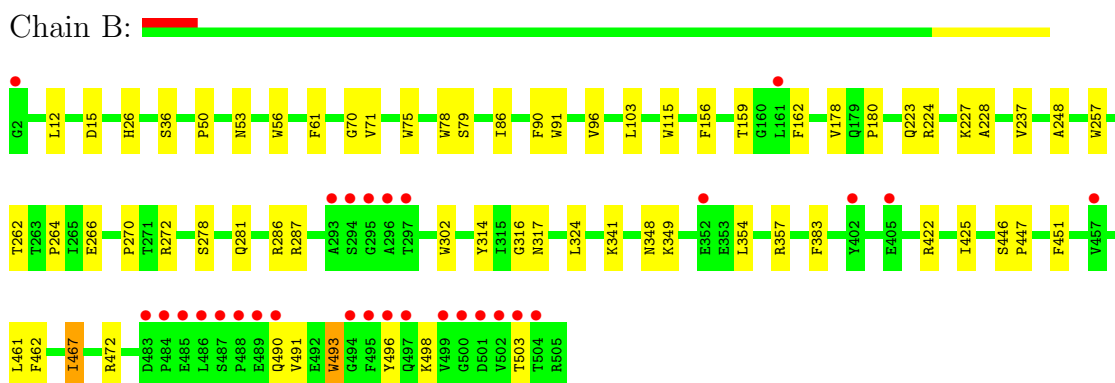
- Molecule 1: Photosystem Q(B) protein



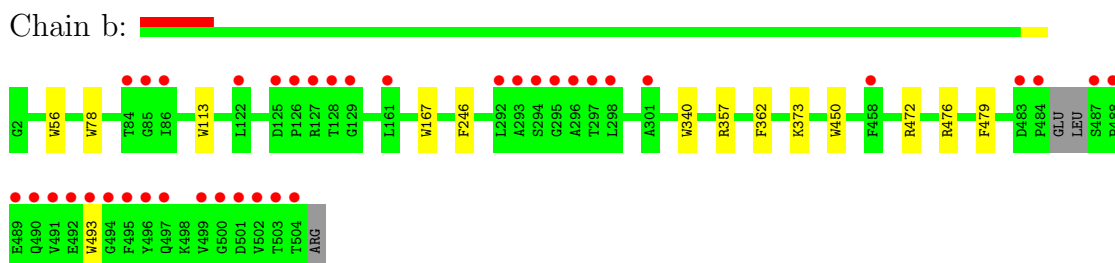
- Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

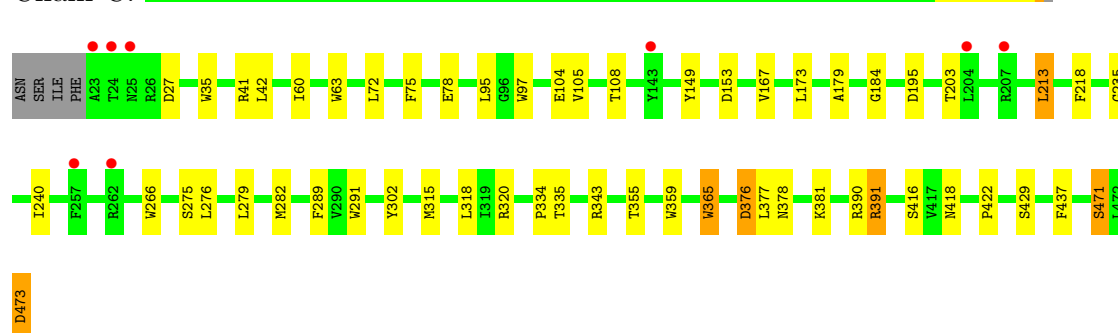


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein



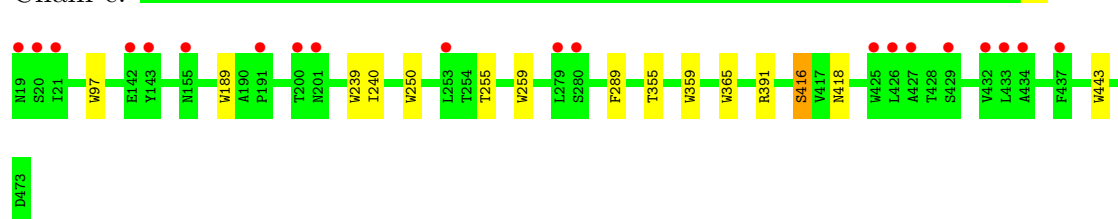
- Molecule 3: Photosystem II 44 kDa reaction center protein

Chain C:



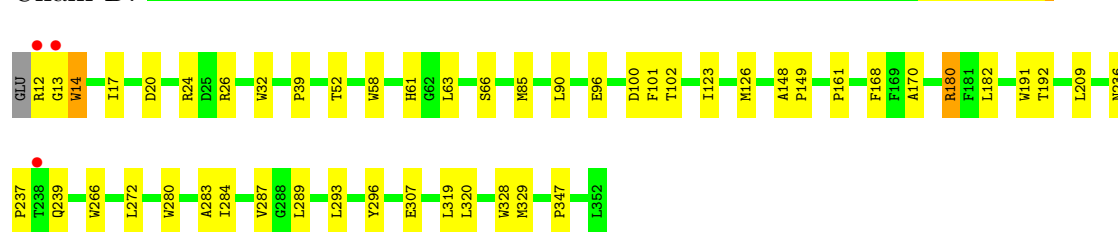
- Molecule 3: Photosystem II 44 kDa reaction center protein

Chain c:



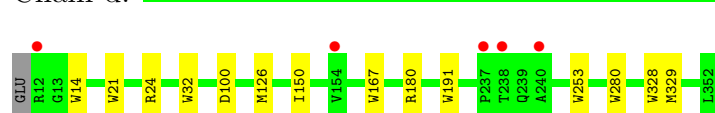
- Molecule 4: Photosystem II D2 protein

Chain D:



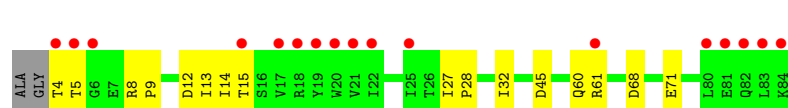
- Molecule 4: Photosystem II D2 protein

Chain d:



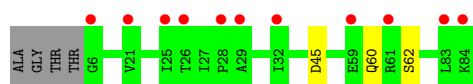
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:



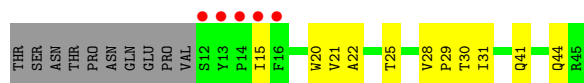
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:



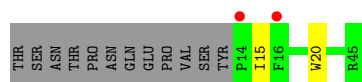
- Molecule 6: Cytochrome b559 subunit beta

Chain F:



- Molecule 6: Cytochrome b559 subunit beta

Chain f:



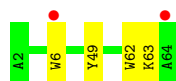
- Molecule 7: Photosystem II reaction center protein H

Chain H:



- Molecule 7: Photosystem II reaction center protein H

Chain h:



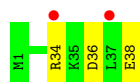
- Molecule 8: Photosystem II reaction center protein I

Chain I:



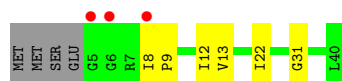
- Molecule 8: Photosystem II reaction center protein I

Chain i:



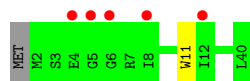
- Molecule 9: Photosystem II reaction center protein J

Chain J:



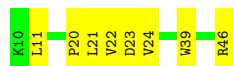
- Molecule 9: Photosystem II reaction center protein J

Chain j: 



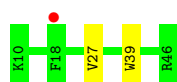
- Molecule 10: Photosystem II reaction center protein K

Chain K: 



- Molecule 10: Photosystem II reaction center protein K

Chain k: 



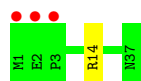
- Molecule 11: Photosystem II reaction center protein L

Chain L: 



- Molecule 11: Photosystem II reaction center protein L

Chain l: 



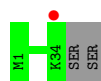
- Molecule 12: Photosystem II reaction center protein M

Chain M: 



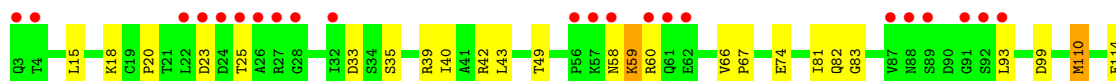
- Molecule 12: Photosystem II reaction center protein M

Chain m: 



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

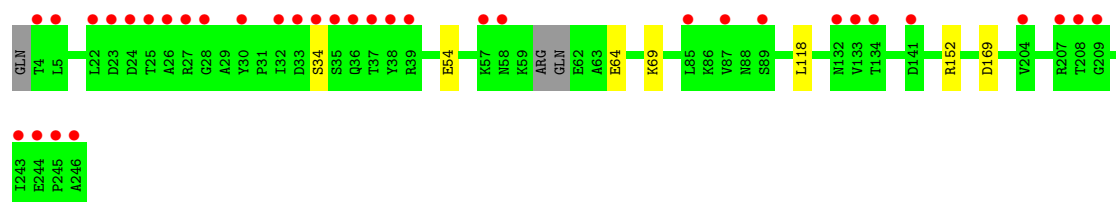
Chain O: 





- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



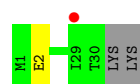
- Molecule 14: Photosystem II reaction center protein T

Chain T:



- Molecule 14: Photosystem II reaction center protein T

Chain t:



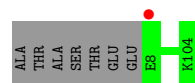
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



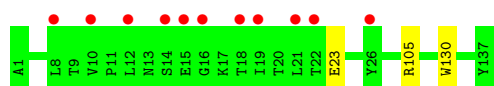
- Molecule 16: Cytochrome c-550

Chain V:



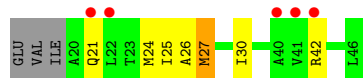
- Molecule 16: Cytochrome c-550

Chain v:



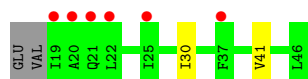
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



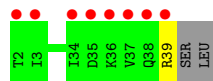
- Molecule 18: Photosystem II reaction center protein X

Chain X:



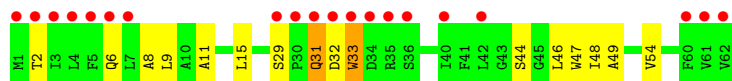
- Molecule 18: Photosystem II reaction center protein X

Chain x:



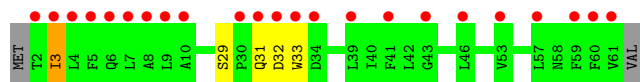
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:



- Molecule 19: Photosystem II reaction center protein Z

Chain 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)	20.00 – 1.90 49.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.90) 99.8 (49.02-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.194 0.157 , 0.194	Depositor DCC
R_{free} test set	31215 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 623234 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54036	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, BCT, BCR, DGD, HSK, FE2, RRX, LHG, GOL, CL, CA, CLA, SO4, HEM, FME, UNL, HTG, MG, OEX, PHO, LMT, 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	1.08	4/2730 (0.1%)	0.90	1/3723 (0.0%)
1	a	1.06	9/2721 (0.3%)	0.86	4/3711 (0.1%)
2	B	1.03	9/4179 (0.2%)	0.89	5/5693 (0.1%)
2	b	1.01	7/4134 (0.2%)	0.85	2/5633 (0.0%)
3	C	1.00	7/3624 (0.2%)	0.84	9/4933 (0.2%)
3	c	0.96	8/3662 (0.2%)	0.81	0/4986
4	D	1.13	5/2804 (0.2%)	0.93	3/3820 (0.1%)
4	d	1.05	8/2825 (0.3%)	0.87	2/3847 (0.1%)
5	E	0.81	0/676	0.82	0/924
5	e	0.81	0/658	0.78	1/899 (0.1%)
6	F	0.90	1/283 (0.4%)	0.71	0/386
6	f	0.92	1/265 (0.4%)	0.69	0/360
7	H	0.98	1/511 (0.2%)	0.79	0/697
7	h	0.94	2/511 (0.4%)	0.81	0/697
8	I	0.77	0/291	0.78	0/394
8	i	0.75	0/308	0.77	0/415
9	J	0.94	0/257	0.68	0/349
9	j	0.81	1/277 (0.4%)	0.69	0/376
10	K	0.76	1/303 (0.3%)	0.75	0/418
10	k	0.79	1/296 (0.3%)	0.77	0/408
11	L	1.05	0/312	0.88	0/425
11	l	1.00	0/313	0.84	1/428 (0.2%)
12	M	0.85	0/257	0.91	0/352
12	m	0.86	0/270	0.80	0/370
13	O	0.84	0/1924	0.89	0/2610
13	o	0.79	0/1900	0.86	3/2577 (0.1%)
14	T	0.93	0/255	0.86	0/346
14	t	0.99	0/255	0.92	0/346
15	U	0.93	0/781	0.90	1/1059 (0.1%)
15	u	0.95	0/786	0.91	0/1067
16	V	0.97	0/1093	0.89	1/1485 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.88	1/1084 (0.1%)	0.85	1/1475 (0.1%)
17	Y	0.55	0/197	0.66	0/263
17	y	0.50	0/197	0.75	0/264
18	X	0.72	0/286	0.75	0/387
18	x	0.67	0/286	0.75	0/387
19	Z	0.76	2/470 (0.4%)	0.74	0/645
19	z	0.68	1/442 (0.2%)	0.71	0/608
All	All	0.97	69/42423 (0.2%)	0.85	34/57763 (0.1%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	TRP	CD2-CE2	7.33	1.50	1.41
7	H	62	TRP	CD2-CE2	6.81	1.49	1.41
3	c	443	TRP	CD2-CE2	6.79	1.49	1.41
1	A	284	TRP	CD2-CE2	6.79	1.49	1.41
3	C	359	TRP	CD2-CE2	6.46	1.49	1.41
4	d	328	TRP	CD2-CE2	6.33	1.49	1.41
9	j	11	TRP	CD2-CE2	6.32	1.49	1.41
1	A	20	TRP	CD2-CE2	6.16	1.48	1.41
19	Z	33	TRP	CD2-CE2	6.13	1.48	1.41
4	D	328	TRP	CD2-CE2	6.13	1.48	1.41
2	b	113	TRP	CD2-CE2	6.00	1.48	1.41
3	c	189	TRP	CD2-CE2	5.95	1.48	1.41
4	d	167	TRP	CD2-CE2	5.94	1.48	1.41
2	B	56	TRP	CD2-CE2	5.94	1.48	1.41
16	v	130	TRP	CD2-CE2	5.86	1.48	1.41
7	h	6	TRP	CD2-CE2	5.79	1.48	1.41
2	b	340	TRP	CD2-CE2	5.75	1.48	1.41
3	c	239	TRP	CD2-CE2	5.75	1.48	1.41
10	k	39	TRP	CD2-CE2	5.74	1.48	1.41
6	F	20	TRP	CD2-CE2	5.66	1.48	1.41
2	B	75	TRP	CD2-CE2	5.66	1.48	1.41
6	f	20	TRP	CD2-CE2	5.65	1.48	1.41
1	a	32	TRP	CD2-CE2	5.63	1.48	1.41
4	D	32	TRP	CD2-CE2	5.62	1.48	1.41
1	a	161	TYR	CE1-CZ	5.59	1.45	1.38
19	z	33	TRP	CD2-CE2	5.56	1.48	1.41
7	h	62	TRP	CD2-CE2	5.55	1.48	1.41
3	c	365	TRP	CD2-CE2	5.53	1.48	1.41
4	d	21	TRP	CD2-CE2	5.53	1.48	1.41
19	Z	47	TRP	CD2-CE2	5.50	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	365	TRP	CD2-CE2	5.47	1.48	1.41
3	c	97	TRP	CD2-CE2	5.44	1.47	1.41
4	d	253	TRP	CD2-CE2	5.43	1.47	1.41
2	B	91	TRP	CD2-CE2	5.41	1.47	1.41
1	a	131	TRP	CD2-CE2	5.41	1.47	1.41
1	a	20	TRP	CD2-CE2	5.40	1.47	1.41
3	C	35	TRP	CD2-CE2	5.38	1.47	1.41
2	b	450	TRP	CD2-CE2	5.34	1.47	1.41
3	C	291	TRP	CD2-CE2	5.30	1.47	1.41
2	B	302	TRP	CD2-CE2	5.30	1.47	1.41
2	B	56	TRP	CG-CD1	5.29	1.44	1.36
2	b	56	TRP	CD2-CE2	5.28	1.47	1.41
1	a	142	TRP	CD2-CE2	5.27	1.47	1.41
3	c	259	TRP	CD2-CE2	5.26	1.47	1.41
4	D	58	TRP	CD2-CE2	5.26	1.47	1.41
2	B	115	TRP	CD2-CE2	5.26	1.47	1.41
3	c	250	TRP	CD2-CE2	5.24	1.47	1.41
2	b	78	TRP	CD2-CE2	5.23	1.47	1.41
3	C	97	TRP	CD2-CE2	5.23	1.47	1.41
1	a	105	TRP	CD2-CE2	5.22	1.47	1.41
2	B	493	TRP	CD2-CE2	5.21	1.47	1.41
4	d	32	TRP	CD2-CE2	5.20	1.47	1.41
2	b	493	TRP	CD2-CE2	5.18	1.47	1.41
3	C	266	TRP	CD2-CE2	5.16	1.47	1.41
3	C	63	TRP	CD2-CE2	5.13	1.47	1.41
2	b	167	TRP	CD2-CE2	5.12	1.47	1.41
4	D	280	TRP	CD2-CE2	5.12	1.47	1.41
2	B	257	TRP	CD2-CE2	5.11	1.47	1.41
10	K	39	TRP	CD2-CE2	5.10	1.47	1.41
4	D	14	TRP	CD2-CE2	5.10	1.47	1.41
4	d	280	TRP	CD2-CE2	5.09	1.47	1.41
1	A	278	TRP	CD2-CE2	5.08	1.47	1.41
1	a	169	SER	CA-CB	5.08	1.60	1.52
4	d	191	TRP	CD2-CE2	5.06	1.47	1.41
1	A	80	GLY	N-CA	5.05	1.53	1.46
1	a	317	TRP	CD2-CE2	5.05	1.47	1.41
3	c	359	TRP	CD2-CE2	5.03	1.47	1.41
1	a	278	TRP	CD2-CE2	5.02	1.47	1.41
4	d	14	TRP	CD2-CE2	5.02	1.47	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	272	ARG	NE-CZ-NH1	-7.88	116.36	120.30
13	o	152	ARG	NE-CZ-NH1	-7.53	116.54	120.30
2	B	357	ARG	NE-CZ-NH2	-7.36	116.62	120.30
3	C	153	ASP	CB-CG-OD1	7.03	124.63	118.30
4	D	100	ASP	CB-CG-OD2	7.02	124.62	118.30
3	C	153	ASP	CB-CG-OD2	-6.97	112.03	118.30
4	d	100	ASP	CB-CG-OD1	6.87	124.48	118.30
5	e	45	ASP	CB-CG-OD1	6.45	124.11	118.30
15	U	39	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	C	195	ASP	CB-CG-OD1	-6.39	112.55	118.30
3	C	195	ASP	CB-CG-OD2	6.16	123.84	118.30
1	a	342	ASP	CB-CG-OD1	6.08	123.77	118.30
3	C	343	ARG	NE-CZ-NH2	-5.91	117.34	120.30
3	C	473	ASP	CB-CG-OD2	5.88	123.60	118.30
4	D	329	MET	CG-SD-CE	5.83	109.54	100.20
16	v	105	ARG	NE-CZ-NH1	-5.83	117.38	120.30
2	b	357	ARG	NE-CZ-NH2	-5.67	117.46	120.30
13	o	169	ASP	CB-CG-OD2	5.67	123.41	118.30
13	o	69	LYS	CD-CE-NZ	-5.63	98.75	111.70
11	l	14	ARG	NE-CZ-NH1	-5.58	117.51	120.30
2	B	287[A]	ARG	NE-CZ-NH2	-5.57	117.51	120.30
2	B	287[B]	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	a	131	TRP	CA-CB-CG	-5.42	103.40	113.70
1	a	269	ARG	NE-CZ-NH2	-5.41	117.59	120.30
3	C	213	LEU	CB-CG-CD1	-5.40	101.82	111.00
4	d	126	MET	CG-SD-CE	-5.36	91.62	100.20
1	a	342	ASP	CB-CG-OD2	-5.29	113.54	118.30
2	B	15	ASP	CB-CG-OD1	5.26	123.04	118.30
3	C	376	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	131	TRP	CA-CB-CG	-5.26	103.71	113.70
4	D	26	ARG	NE-CZ-NH2	-5.24	117.68	120.30
16	V	99	ASP	CB-CG-OD1	5.17	122.95	118.30
3	C	27	ASP	CB-CG-OD1	5.16	122.94	118.30
2	b	357	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2633	0	2544	37	0
1	a	2625	0	2538	0	0
2	B	4009	0	3879	59	0
2	b	3964	0	3817	0	0
3	C	3502	0	3431	43	0
3	c	3536	0	3460	0	0
4	D	2726	0	2618	45	0
4	d	2741	0	2643	0	0
5	E	657	0	637	22	0
5	e	639	0	617	0	0
6	F	274	0	279	7	0
6	f	257	0	269	0	0
7	H	498	0	518	7	0
7	h	498	0	518	0	0
8	I	294	0	304	6	0
8	i	311	0	326	0	0
9	J	251	0	257	5	0
9	j	271	0	270	0	0
10	K	290	0	294	7	0
10	k	286	0	285	0	0
11	L	302	0	316	7	0
11	l	300	0	314	0	0
12	M	261	0	280	21	0
12	m	271	0	293	0	0
13	O	1878	0	1853	34	0
13	o	1855	0	1823	0	0
14	T	256	0	256	4	0
14	t	256	0	256	0	0
15	U	770	0	769	6	0
15	u	772	0	766	0	0
16	V	1066	0	1075	12	0
16	v	1060	0	1053	0	0
17	Y	196	0	219	8	0
17	y	196	0	208	0	0
18	X	280	0	312	9	0
18	x	280	0	312	0	0
19	Z	459	0	484	7	0
19	z	431	0	438	0	0
20	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	a	2	0	0	0	0
23	A	260	0	288	10	0
23	B	1040	0	1152	60	0
23	C	845	0	936	36	0
23	D	130	0	144	7	0
23	a	260	0	288	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	128	0	148	5	0
24	a	128	0	148	0	0
25	A	40	0	56	2	0
25	B	120	0	168	5	0
25	C	80	0	112	5	0
25	D	40	0	56	5	0
25	K	80	0	112	9	0
25	T	40	0	56	9	0
25	a	40	0	56	0	0
25	b	120	0	168	0	0
25	c	80	0	112	0	0
25	d	40	0	56	0	0
25	k	80	0	112	0	0
25	t	40	0	56	0	0
26	A	108	0	155	5	0
26	B	54	0	78	5	0
26	D	45	0	57	3	0
26	L	54	0	78	5	0
26	a	108	0	156	0	0
26	f	33	0	39	0	0
27	A	51	0	72	3	0
27	B	51	0	72	4	0
27	C	51	0	72	2	0
27	D	51	0	72	2	0
27	Z	51	0	72	0	0
27	a	51	0	72	0	0
27	b	51	0	72	0	0
27	c	102	0	144	0	0
27	d	51	0	72	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A	55	0	80	10	0
28	D	55	0	80	0	0
28	a	55	0	80	0	0
28	d	55	0	80	0	0
29	A	69	0	0	0	0
29	B	56	0	0	4	0
29	C	34	0	0	0	0
29	D	56	0	0	2	0
29	E	27	0	0	0	0
29	H	10	0	0	0	0
29	I	24	0	0	0	0
29	J	26	0	0	0	0
29	L	14	0	0	1	0
29	M	16	0	0	1	0
29	T	13	0	0	0	0
29	X	16	0	0	1	0
29	Z	16	0	0	0	0
29	a	56	0	0	0	0
29	b	84	0	0	0	0
29	c	40	0	0	0	0
29	d	16	0	0	0	0
29	e	11	0	0	0	0
29	i	55	0	0	0	0
29	j	28	0	0	0	0
29	t	16	0	0	0	0
29	x	16	0	0	0	0
29	z	16	0	0	0	0
30	A	35	0	46	0	0
30	B	35	0	46	4	0
30	C	35	0	46	4	0
30	F	35	0	46	0	0
30	J	24	0	35	1	0
30	M	70	0	92	3	0
30	Z	35	0	46	3	0
30	a	35	0	46	0	0
30	b	49	0	70	0	0
30	c	35	0	46	0	0
30	m	70	0	92	0	0
30	t	24	0	35	0	0
30	z	32	0	36	0	0
31	A	18	0	22	4	0
31	B	36	0	48	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	C	18	0	24	4	0
31	D	6	0	8	3	0
31	L	6	0	8	1	0
31	O	6	0	8	0	0
31	V	18	0	24	0	0
31	a	18	0	24	0	0
31	b	30	0	40	0	0
31	c	24	0	32	0	0
31	f	6	0	6	0	0
31	h	6	0	8	0	0
31	l	6	0	8	0	0
31	v	18	0	24	0	0
32	B	1	0	0	0	0
32	F	1	0	0	0	0
32	O	1	0	0	0	0
32	b	1	0	0	0	0
32	c	1	0	0	0	0
32	f	1	0	0	0	0
32	o	1	0	0	0	0
33	B	95	0	130	3	0
33	C	38	0	52	1	0
33	D	19	0	26	2	0
33	O	19	0	26	0	0
33	U	9	0	15	1	0
33	V	13	0	11	0	0
33	b	76	0	104	0	0
33	c	38	0	52	0	0
33	d	19	0	26	0	0
33	u	14	0	19	0	0
34	C	186	0	246	2	0
34	D	53	0	71	9	0
34	H	62	0	82	1	0
34	c	186	0	246	0	0
34	d	50	0	69	0	0
34	h	62	0	82	0	0
35	D	4	0	0	0	0
35	a	4	0	0	0	0
36	D	144	0	213	24	0
36	E	49	0	74	3	0
36	L	49	0	74	2	0
36	a	40	0	53	0	0
36	d	147	0	222	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	l	49	0	74	0	0
37	F	43	0	30	4	0
37	V	43	0	30	1	0
37	f	43	0	30	0	0
37	v	43	0	30	0	0
38	H	41	0	0	1	0
38	h	41	0	0	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	O	5	0	0	0	0
41	A	170	0	0	1	0
41	B	319	0	0	4	0
41	C	263	0	0	4	0
41	D	161	0	0	2	0
41	E	35	0	0	4	0
41	F	12	0	0	0	0
41	H	52	0	0	0	0
41	I	8	0	0	0	0
41	J	9	0	0	0	0
41	K	8	0	0	1	0
41	L	24	0	0	0	0
41	M	16	0	0	1	0
41	O	202	0	0	5	1
41	T	10	0	0	0	0
41	U	100	0	0	2	0
41	V	144	0	0	3	0
41	X	14	0	0	0	0
41	Y	6	0	0	0	0
41	Z	1	0	0	0	0
41	a	155	0	0	0	0
41	b	306	0	0	0	0
41	c	245	0	0	0	1
41	d	160	0	0	0	0
41	e	22	0	0	0	0
41	f	14	0	0	0	0
41	h	53	0	0	0	0
41	i	14	0	0	0	0
41	j	9	0	0	0	0
41	k	5	0	0	0	0
41	l	18	0	0	0	0
41	m	16	0	0	0	0
41	o	175	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	t	12	0	0	0	0
41	u	106	0	0	0	0
41	v	104	0	0	0	0
41	x	6	0	0	0	0
41	y	7	0	0	0	0
41	z	2	0	0	0	0
All	All	54036	0	51643	458	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (458) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:M:16[A]:LEU:CD2	12:M:16[A]:LEU:HD23	0.97	1.49
12:M:16[A]:LEU:CD2	12:M:16[A]:LEU:CD2	0.00	1.21
36:D:409:LHG:H112	36:D:409:LHG:C38	13.80	1.17
26:L:103:SQD:H1	26:L:103:SQD:H462	1.28	1.12
36:D:409:LHG:H372	36:D:409:LHG:H131	13.21	1.10
1:A:214:MET:CG	28:A:414:PL9:H102	1.84	1.07
5:E:9:PRO:HA	36:E:101:LHG:HC32	1.32	1.07
1:A:214:MET:HG2	28:A:414:PL9:C10	1.84	1.06
36:D:409:LHG:H112	36:D:409:LHG:H381	14.54	1.04
13:O:33:ASP:OD1	13:O:35:SER:HB3	3.18	1.01
30:C:520:LMT:H6'1	8:I:26:GLY:HA3	1.42	0.99
26:B:621:SQD:H462	26:B:621:SQD:H1	1.44	0.99
12:M:16[A]:LEU:HD23	12:M:16[A]:LEU:HD21	1.58	0.99
31:C:524:GOL:H11	41:C:706:HOH:O	1.63	0.98
36:D:410:LHG:H152	36:D:410:LHG:C33	1.94	0.98
15:U:86:GLU:H	15:U:86:GLU:CD	1.66	0.97
23:B:615:CLA:H18	27:B:622:LMG:H421	1.46	0.96
1:A:214:MET:HG2	28:A:414:PL9:H102	0.98	0.96
23:B:617:CLA:C19	29:B:627:UNL:C16	2.43	0.96
23:C:509:CLA:HBB1	23:C:509:CLA:HMB1	1.48	0.94
31:A:423:GOL:H11	12:M:1:FME:HG2	59.12	0.90
36:D:410:LHG:H152	36:D:410:LHG:H332	1.54	0.89
12:M:16[A]:LEU:HD23	12:M:16[A]:LEU:HD23	0.00	0.88
5:E:68:ASP:OD1	5:E:71:GLU:HB2	1.75	0.87
12:M:16[A]:LEU:HD21	12:M:16[A]:LEU:HG	2.34	0.86
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.88	0.86
4:D:236:ASN:O	4:D:239:GLN:HG2	2.38	0.86
23:B:617:CLA:H191	29:B:627:UNL:C16	2.05	0.86
5:E:9:PRO:HA	36:E:101:LHG:C3	2.06	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:B:612:CLA:HMB1	23:B:612:CLA:HBB1	1.58	0.85
26:L:103:SQD:C1	26:L:103:SQD:H462	2.06	0.84
23:D:403:CLA:HBB1	23:D:403:CLA:HMB1	1.80	0.83
23:C:504:CLA:H201	36:D:410:LHG:C35	2.08	0.82
13:O:179:GLU:HG2	41:O:569:HOH:O	1.82	0.80
36:D:410:LHG:H152	36:D:410:LHG:H331	1.62	0.79
5:E:45:ASP:OD1	41:E:228[A]:HOH:O	1.99	0.79
25:T:101:BCR:HC8	25:T:101:BCR:H321	1.65	0.78
4:D:102:THR:OG1	34:D:406:DGD:HG31	1.82	0.78
3:C:279:LEU:HD12	3:C:282:MET:CE	2.33	0.78
12:M:16[A]:LEU:HD21	12:M:16[A]:LEU:CG	2.06	0.78
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.66	0.76
41:B:799:HOH:O	13:O:58:ASN:HA	64.81	0.76
31:D:415:GOL:H11	12:M:1:FME:HG2	1.67	0.75
36:D:409:LHG:H372	36:D:409:LHG:C13	12.99	0.75
36:D:409:LHG:H322	36:D:409:LHG:H151	7.02	0.75
2:B:503:THR:O	18:X:39:ARG:HG2	2.27	0.75
26:L:103:SQD:H371	29:M:103:UNL:C16	2.17	0.75
23:B:614:CLA:HBB1	23:B:614:CLA:HMB1	1.70	0.74
23:C:504:CLA:H191	36:D:410:LHG:C35	2.17	0.73
4:D:13:GLY:HA3	33:D:414:HTG:H62	1.69	0.73
23:C:512:CLA:HMB1	23:C:512:CLA:HBB1	1.71	0.73
23:C:506:CLA:HMC2	23:C:507:CLA:H102	1.71	0.73
23:A:406:CLA:HBB1	23:A:406:CLA:HMB1	1.71	0.72
2:B:462:PHE:CZ	23:B:616:CLA:HMB3	24.25	0.71
13:O:58:ASN:C	13:O:60:ARG:H	1.94	0.71
12:M:16[A]:LEU:CD2	12:M:16[A]:LEU:HD21	0.97	0.71
23:B:616:CLA:HMB1	23:B:616:CLA:HBB1	1.90	0.70
23:B:617:CLA:HED2	23:B:617:CLA:H43	1.73	0.70
23:A:405:CLA:HBB1	23:A:405:CLA:HMB1	1.72	0.70
26:B:621:SQD:C46	26:B:621:SQD:H1	2.21	0.70
36:D:409:LHG:C11	36:D:409:LHG:C38	14.58	0.70
23:B:617:CLA:H193	29:B:627:UNL:C16	2.22	0.70
23:B:606:CLA:C14	23:B:611:CLA:HED2	2.22	0.69
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.75	0.69
12:M:16[A]:LEU:CD2	12:M:16[A]:LEU:CG	1.52	0.69
34:D:406:DGD:HD4	5:E:45:ASP:HB3	1.73	0.69
16:V:2:GLU:HB2	41:V:384:HOH:O	40.09	0.69
3:C:72:LEU:HD11	3:C:108:THR:HB	2.39	0.68
3:C:320:ARG:HG3	31:C:524:GOL:H2	1.75	0.68
34:D:406:DGD:HD3	5:E:45:ASP:HB3	3.03	0.68
13:O:74[A]:GLU:OE1	41:O:550:HOH:O	2.11	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:183:MET:HA	23:A:405:CLA:HMD2	1.76	0.68
5:E:61:ARG:O	41:E:214[A]:HOH:O	2.10	0.67
34:D:406:DGD:O1B	34:D:406:DGD:O2D	2.13	0.67
5:E:60:GLN:O	41:E:214[B]:HOH:O	2.12	0.66
1:A:248[A]:ILE:HD11	4:D:237:PRO:O	1.96	0.66
1:A:248[A]:ILE:HD13	1:A:249:VAL:H	1.59	0.66
25:D:404:BCR:H313	34:D:406:DGD:HAW1	5.23	0.66
28:A:414:PL9:H403	6:F:22:ALA:HB2	1.78	0.65
23:B:611:CLA:HBB1	23:B:611:CLA:HHC	1.77	0.65
23:C:506:CLA:H18	23:C:506:CLA:H122	1.76	0.65
15:U:86:GLU:N	15:U:86:GLU:CD	2.46	0.65
25:K:102:BCR:C8	25:K:102:BCR:H331	2.25	0.65
23:C:511:CLA:HBB1	23:C:511:CLA:HMB1	1.78	0.65
4:D:14:TRP:CD1	33:D:414:HTG:H61	2.32	0.65
13:O:82:GLN:NE2	41:O:563:HOH:O	2.29	0.65
25:C:515:BCR:C8	25:C:515:BCR:H331	2.25	0.64
8:I:35:LYS:HB2	8:I:35:LYS:NZ	4.94	0.64
23:B:615:CLA:HBB1	23:B:615:CLA:HMB1	2.16	0.64
30:M:101:LMT:O6'	41:M:211[B]:HOH:O	2.15	0.64
4:D:85:MET:HE1	4:D:96:GLU:HG2	2.15	0.63
2:B:462:PHE:CE1	23:B:616:CLA:HMB3	23.63	0.63
10:K:24[A]:VAL:HG13	17:Y:25:ILE:HD13	1.81	0.62
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.33	0.62
23:C:506:CLA:HBB1	23:C:506:CLA:HMB1	1.81	0.62
13:O:203:LYS:HE3	41:O:584:HOH:O	2.00	0.62
4:D:85:MET:CE	4:D:96:GLU:HG2	2.53	0.62
26:B:621:SQD:H45	14:T:23:PHE:CD1	36.10	0.62
19:Z:15:LEU:HD22	19:Z:46:LEU:HD23	2.77	0.62
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.17	0.62
23:C:508:CLA:HBB1	23:C:508:CLA:HMB1	1.82	0.61
11:L:24[A]:ILE:CD1	12:M:18:PRO:HB2	2.30	0.61
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.35	0.61
23:A:410:CLA:HBB1	23:A:410:CLA:HMB1	2.12	0.61
24:A:409:PHO:HBB1	24:A:409:PHO:HMB1	1.83	0.61
10:K:24[A]:VAL:CG1	17:Y:25:ILE:HD13	2.31	0.61
9:J:9:PRO:HD2	9:J:12:ILE:HD12	2.09	0.60
31:A:423:GOL:H11	12:M:1:FME:CG	59.33	0.60
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.35	0.60
13:O:33:ASP:C	13:O:35:SER:H	2.60	0.60
4:D:272:LEU:C	4:D:272:LEU:HD23	2.36	0.60
23:C:513:CLA:HMB1	23:C:513:CLA:HBB1	1.83	0.59
25:D:404:BCR:C8	25:D:404:BCR:H331	2.41	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:B:617:CLA:HMB1	23:B:617:CLA:HBB1	1.84	0.59
13:O:66:VAL:HB	13:O:67:PRO:HD2	1.99	0.59
13:O:42:ARG:O	13:O:241:ALA:HA	2.19	0.59
23:B:607:CLA:H43	23:B:608:CLA:H2	25.33	0.59
30:B:623:LMT:H122	29:D:412:UNL:C22	2.33	0.59
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.59
2:B:103:LEU:HD21	23:B:606:CLA:HMC3	1.84	0.58
2:B:467:ILE:HG13	4:D:126:MET:CE	2.33	0.58
26:A:412:SQD:H383	9:J:22:ILE:HD11	1.86	0.58
3:C:318:LEU:C	3:C:318:LEU:HD23	2.27	0.58
25:K:101:BCR:HC8	25:K:101:BCR:H321	1.90	0.58
5:E:61:ARG:HG3	41:E:214[B]:HOH:O	2.04	0.58
30:C:520:LMT:C6B	8:I:26:GLY:HA3	2.28	0.58
25:K:102:BCR:HC8	25:K:102:BCR:H331	1.86	0.58
1:A:259:ILE:HD12	28:A:414:PL9:C25	2.34	0.57
13:O:129:THR:HA	13:O:141:ASP:O	2.25	0.57
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.75	0.57
5:E:15:THR:HB	9:J:8:ILE:O	2.04	0.57
25:T:101:BCR:H23C	25:T:101:BCR:H382	1.87	0.57
30:C:520:LMT:H6'1	8:I:26:GLY:CA	2.27	0.56
4:D:12:ARG:HG3	4:D:17:ILE:HD11	4.27	0.56
23:A:410:CLA:H91	30:C:520:LMT:H123	1.88	0.56
24:A:408:PHO:HBB1	24:A:408:PHO:HMB1	1.87	0.56
30:Z:102:LMT:O3'	30:Z:102:LMT:H2B	2.05	0.56
34:D:406:DGD:HB21	34:D:406:DGD:HA22	1.86	0.56
19:Z:44:SER:O	19:Z:48:ILE:HG13	2.35	0.56
15:U:86:GLU:HG2	41:U:328:HOH:O	7.42	0.55
13:O:207:ARG:NH1	41:O:536:HOH:O	31.84	0.55
23:C:502:CLA:H193	33:C:521:HTG:H3'1	1.87	0.55
2:B:462:PHE:CE1	23:B:614:CLA:HMB3	2.42	0.55
3:C:203:THR:O	3:C:235:GLY:HA3	2.22	0.55
2:B:50:PRO:HB2	31:B:633:GOL:H12	26.53	0.55
3:C:279:LEU:HD22	23:C:509:CLA:HED2	1.89	0.55
3:C:391[A]:ARG:HD3	41:C:825[A]:HOH:O	2.05	0.54
36:D:410:LHG:H342	36:D:410:LHG:H302	1.89	0.54
23:C:513:CLA:HMD1	30:Z:102:LMT:H5'	1.88	0.54
23:B:612:CLA:H142	36:L:101:LHG:H361	1.90	0.54
31:A:423:GOL:C1	12:M:1:FME:HG2	59.91	0.54
2:B:446:SER:HB2	2:B:447:PRO:CD	2.35	0.54
6:F:15:ILE:HD12	6:F:15:ILE:H	4.07	0.54
41:B:956:HOH:O	12:M:6:LEU:HD12	28.85	0.54
25:K:101:BCR:C8	25:K:101:BCR:H311	2.37	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
33:U:201:HTG:H1'1	41:U:372:HOH:O	2.07	0.54
15:U:73:GLN:O	15:U:77:GLU:HG3	2.07	0.54
23:B:605:CLA:HMB1	23:B:605:CLA:HBB1	1.88	0.53
3:C:376:ASP:OD1	3:C:378[A]:ASN:HB3	2.08	0.53
23:B:607:CLA:HMD2	23:B:615:CLA:H203	35.85	0.53
4:D:123:ILE:HD11	34:H:102:DGD:HAE1	1.89	0.53
2:B:26:HIS:HB2	23:B:613:CLA:HMB2	1.90	0.53
2:B:237:VAL:HG12	23:B:615:CLA:HMD1	24.54	0.53
3:C:167:VAL:HG21	23:C:512:CLA:HHB	1.91	0.53
4:D:307:GLU:HG3	41:D:611:HOH:O	34.46	0.53
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
5:E:28:PRO:O	5:E:32:ILE:HG12	2.09	0.52
23:B:613:CLA:H203	23:B:613:CLA:H152	5.89	0.52
23:D:403:CLA:H192	18:X:15[A]:LEU:HD11	1.92	0.52
2:B:341:LYS:HZ1	33:B:626:HTG:C2	54.30	0.52
28:A:414:PL9:H502	4:D:39:PRO:HG3	1.91	0.52
3:C:429:SER:HB3	34:C:517:DGD:HBT2	1.92	0.52
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.06	0.52
26:A:412:SQD:H141	36:D:410:LHG:H172	1.91	0.52
23:A:407:CLA:HMD3	4:D:182:LEU:HD11	1.91	0.52
2:B:341:LYS:NZ	33:B:626:HTG:O2	54.23	0.52
23:C:501:CLA:H42	23:C:502:CLA:HMD1	1.91	0.52
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.52
31:D:415:GOL:C1	12:M:1:FME:HG2	2.38	0.51
2:B:223[A]:GLN:NE2	2:B:227:LYS:HD2	2.24	0.51
25:B:619:BCR:C8	25:B:619:BCR:H331	2.39	0.51
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.93	0.51
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.44	0.51
16:V:55[B]:ARG:NH1	41:V:357:HOH:O	22.75	0.51
2:B:266:GLU:HB3	31:B:635:GOL:H31	1.92	0.51
2:B:286:ARG:HH11	2:B:286:ARG:HG2	1.76	0.51
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.91	0.51
4:D:266:TRP:CD1	36:D:408:LHG:HC31	9.37	0.51
13:O:49[B]:THR:OG1	13:O:236:GLN:HB2	2.11	0.51
31:C:524:GOL:H12	37:V:201:HEM:HMD1	1.93	0.51
23:B:607:CLA:H202	33:B:631:HTG:H61	1.92	0.51
23:C:510:CLA:H192	23:C:510:CLA:HBC3	1.93	0.51
5:E:8:ARG:HB3	5:E:13:ILE:HD11	1.92	0.51
3:C:334:PRO:HA	13:O:153:THR:OG1	2.11	0.51
23:B:611:CLA:H203	23:B:611:CLA:H151	1.93	0.51
2:B:79:SER:HB3	2:B:86:ILE:HG12	2.06	0.51
10:K:21:LEU:HB2	17:Y:24:MET:HE2	5.96	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:248:ALA:HA	23:B:604:CLA:H42	1.93	0.50
23:C:512:CLA:H121	23:C:513:CLA:H142	1.93	0.50
4:D:102:THR:OG1	34:D:406:DGD:HD1	2.11	0.50
27:C:519:LMG:O10	30:J:102:LMT:H42	2.10	0.50
23:C:505:CLA:HMD2	25:C:515:BCR:H343	1.92	0.50
5:E:27:ILE:HG12	37:F:101:HEM:HMC3	1.92	0.50
7:H:12:ARG:HB3	7:H:13:PRO:HD3	2.27	0.50
13:O:58:ASN:C	13:O:60:ARG:N	2.63	0.50
27:D:411:LMG:H412	6:F:30:THR:HG21	1.93	0.50
3:C:78:GLU:OE2	16:V:106[A]:ASN:ND2	2.34	0.50
3:C:381:LYS:NZ	13:O:99[A]:ASP:OD2	2.32	0.50
16:V:106[B]:ASN:ND2	41:V:432:HOH:O	2.42	0.50
4:D:101:PHE:HB3	34:D:406:DGD:HG2	1.94	0.49
8:I:29:ALA:O	8:I:35:LYS:HG2	2.12	0.49
4:D:236:ASN:OD1	4:D:237:PRO:HD2	2.60	0.49
1:A:11:ALA:HB1	1:A:15:GLU:HB3	1.94	0.49
2:B:162:PHE:O	23:B:609:CLA:HHD	33.29	0.49
2:B:467:ILE:HG13	4:D:126:MET:HE1	1.94	0.49
13:O:23:ASP:HB3	13:O:25:THR:HG23	1.94	0.49
23:A:405:CLA:CBF	23:A:406:CLA:HAC2	2.42	0.49
17:Y:42:ARG:HD2	19:Z:29:SER:OG	4.76	0.49
1:A:96:ILE:HD12	23:A:410:CLA:HMD1	1.94	0.49
27:A:413:LMG:H111	3:C:218:PHE:HE2	1.77	0.49
25:C:514:BCR:C8	25:C:514:BCR:H331	2.43	0.49
2:B:237:VAL:HG11	23:B:613:CLA:H201	12.93	0.49
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.49
2:B:422:ARG:O	2:B:425:ILE:HG12	2.13	0.49
7:H:38:PHE:HB2	38:H:101:RRX:C10	2.57	0.49
4:D:101:PHE:H	34:D:406:DGD:HA22	4.36	0.49
25:K:101:BCR:HC8	25:K:101:BCR:H311	1.95	0.49
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.95	0.49
36:D:409:LHG:H112	36:D:409:LHG:C37	12.95	0.49
11:L:24[A]:ILE:HD13	12:M:18:PRO:HB2	1.93	0.49
16:V:102:PRO:HA	16:V:105:ARG:HG3	2.59	0.49
2:B:324:LEU:HA	4:D:293[A]:LEU:HG	2.13	0.48
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.41	0.48
13:O:33:ASP:O	13:O:35:SER:N	2.92	0.48
3:C:365:TRP:HB3	3:C:391[B]:ARG:HG2	2.24	0.48
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.53	0.48
1:A:263:ALA:HA	36:E:101:LHG:H291	1.95	0.48
18:X:21:LEU:HD11	29:X:101:UNL:C16	3.29	0.48
1:A:63:ILE:HB	3:C:335:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:467:ILE:HG13	4:D:126:MET:HE2	1.95	0.48
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.56	0.48
2:B:12:LEU:HB2	23:B:615:CLA:HMC2	14.44	0.48
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.96	0.48
26:B:621:SQD:O7	11:L:7:ARG:NH1	2.47	0.48
23:B:614:CLA:H72	23:B:614:CLA:H112	1.64	0.47
23:C:503:CLA:HBB1	23:C:503:CLA:HMB1	1.96	0.47
3:C:437:PHE:CE1	23:C:510:CLA:HMB3	2.48	0.47
34:C:517:DGD:HB22	27:C:519:LMG:H302	1.96	0.47
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.47
23:B:609:CLA:HMB1	23:B:609:CLA:HBB1	1.95	0.47
23:B:617:CLA:H171	25:B:620:BCR:H331	1.96	0.47
7:H:39:LEU:C	7:H:39:LEU:HD23	2.49	0.47
24:A:408:PHO:NC	24:A:408:PHO:ND	2.62	0.47
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.78	0.47
26:L:103:SQD:H311	26:L:103:SQD:H341	1.56	0.47
13:O:110:MET:HG3	13:O:114:GLU:HB3	1.95	0.47
13:O:15:LEU:HD23	13:O:18:LYS:HD2	1.95	0.47
13:O:33:ASP:C	13:O:35:SER:N	3.02	0.47
1:A:11:ALA:HA	1:A:15:GLU:OE1	3.48	0.47
31:D:415:GOL:H11	12:M:1:FME:CG	2.39	0.47
12:M:1:FME:HCN	30:M:101:LMT:O6B	18.16	0.47
1:A:248[A]:ILE:HD13	1:A:249:VAL:N	2.26	0.47
23:A:406:CLA:H162	23:A:406:CLA:H203	1.46	0.47
1:A:313:VAL:O	31:A:422:GOL:H31	2.15	0.47
23:C:511:CLA:H191	30:Z:102:LMT:H122	1.97	0.47
3:C:60:ILE:HG22	23:C:503:CLA:HHD	1.97	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.47
23:B:617:CLA:H91	23:B:617:CLA:H112	1.72	0.46
26:A:418:SQD:H212	25:T:101:BCR:H323	1.96	0.46
3:C:437:PHE:CZ	23:C:510:CLA:HMB3	2.50	0.46
2:B:237:VAL:HG12	23:B:613:CLA:HMD1	1.96	0.46
2:B:451:PHE:CZ	23:B:605:CLA:HED1	2.51	0.46
31:C:524:GOL:C1	41:C:706:HOH:O	2.38	0.46
1:A:246:TYR:CZ	1:A:248[A]:ILE:HG22	2.50	0.46
2:B:493:TRP:HB3	5:E:5:THR:HG23	1.97	0.46
11:L:14:ARG:HH12	26:L:103:SQD:H3	1.80	0.46
23:B:602:CLA:HHC	23:B:602:CLA:CBB	2.46	0.46
23:B:613:CLA:H203	23:B:613:CLA:C15	5.02	0.46
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.56	0.46
23:C:504:CLA:C20	36:D:410:LHG:C35	2.87	0.46
25:T:101:BCR:H321	25:T:101:BCR:C8	2.42	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:61:ARG:HH12	16:V:127:GLY:HA3	2.70	0.46
5:E:60:GLN:HB2	5:E:60:GLN:HE21	4.41	0.46
25:T:101:BCR:HC8	25:T:101:BCR:H311	2.18	0.46
23:B:605:CLA:H43	23:B:606:CLA:H2	1.98	0.45
27:B:622:LMG:H242	4:D:284:ILE:HD13	1.97	0.45
6:F:21:VAL:O	6:F:25:THR:HG23	2.39	0.45
25:K:102:BCR:H11C	25:K:102:BCR:H341	1.77	0.45
4:D:283:ALA:O	4:D:287:VAL:HG23	2.16	0.45
4:D:24:ARG:NH2	18:X:35:ASP:O	4.34	0.45
1:A:298:ASN:ND2	41:A:636:HOH:O	33.52	0.45
23:A:405:CLA:HBD	23:A:406:CLA:HAC2	1.98	0.45
3:C:377:LEU:HG	3:C:381:LYS:HE3	3.17	0.45
24:A:409:PHO:HBC2	24:A:409:PHO:HHD	1.98	0.45
36:D:410:LHG:H342	36:D:410:LHG:C30	2.47	0.45
26:A:412:SQD:H181	26:A:412:SQD:H211	1.61	0.45
2:B:71:VAL:HG23	23:B:607:CLA:HMA2	1.97	0.45
23:B:606:CLA:HAB	23:B:608:CLA:H171	34.16	0.45
3:C:318:LEU:O	3:C:318:LEU:HD23	2.30	0.45
3:C:149:TYR:CZ	23:C:509:CLA:H191	2.52	0.45
13:O:58:ASN:O	13:O:60:ARG:N	2.46	0.45
2:B:266:GLU:HB3	31:B:633:GOL:H31	25.17	0.45
23:B:611:CLA:CBB	23:B:611:CLA:HHC	2.45	0.45
25:B:620:BCR:C8	25:B:620:BCR:H331	2.47	0.45
23:C:511:CLA:HBD	23:C:511:CLA:HAA1	1.98	0.45
36:D:410:LHG:H331	36:D:410:LHG:C15	2.40	0.45
2:B:224:ARG:HH21	30:B:623:LMT:H2'	1.82	0.45
2:B:348:ASN:HB3	2:B:354:LEU:HD11	2.18	0.45
2:B:248:ALA:HA	23:B:606:CLA:H42	8.71	0.45
23:D:403:CLA:H161	7:H:37:LEU:HD21	7.82	0.45
8:I:35:LYS:HB2	8:I:35:LYS:HZ2	4.98	0.45
18:X:27:VAL:O	18:X:31:ILE:HG13	2.22	0.45
24:A:409:PHO:NC	24:A:409:PHO:ND	2.65	0.45
4:D:52:THR:O	4:D:66:SER:HA	2.17	0.45
13:O:39:ARG:HG3	13:O:246:ALA:HB2	3.40	0.45
23:B:617:CLA:H62	23:B:617:CLA:H41	3.01	0.44
2:B:461:LEU:HD22	36:D:408:LHG:H301	1.99	0.44
41:C:822:HOH:O	13:O:149:PRO:HB2	2.17	0.44
25:T:101:BCR:C23	25:T:101:BCR:H382	2.53	0.44
4:D:293[B]:LEU:HD23	4:D:293[B]:LEU:HA	2.10	0.44
28:A:414:PL9:H202	28:A:414:PL9:H162	1.98	0.44
23:B:615:CLA:C9	30:M:101:LMT:H112	11.89	0.44
31:L:104:GOL:H2	14:T:25:GLU:HB3	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:39:ARG:HB2	13:O:83:GLY:O	2.17	0.44
13:O:93:LEU:O	13:O:128:SER:HA	2.23	0.44
2:B:36[A]:SER:OG	25:B:619:BCR:H362	2.18	0.44
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.99	0.44
1:A:12:ASN:HB3	1:A:15:GLU:HB3	5.22	0.44
23:B:604:CLA:HMB1	23:B:604:CLA:HBB1	1.99	0.44
3:C:377:LEU:O	3:C:381:LYS:HG3	2.18	0.44
30:B:623:LMT:C12	29:D:412:UNL:C22	2.95	0.44
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.52	0.44
2:B:224:ARG:HD2	41:B:894:HOH:O	2.16	0.44
26:B:621:SQD:H442	26:B:621:SQD:O9	2.18	0.44
4:D:266:TRP:CD1	36:D:409:LHG:HC31	2.53	0.44
6:F:31:ILE:HG13	37:F:101:HEM:HMC1	2.00	0.44
29:B:628:UNL:C6	41:B:913:HOH:O	65.42	0.44
3:C:41:ARG:NH1	23:C:511:CLA:HMD1	2.33	0.44
27:A:413:LMG:H111	3:C:218:PHE:CE2	2.53	0.43
2:B:228:ALA:HB2	30:B:623:LMT:H21	2.00	0.43
23:C:504:CLA:C19	36:D:410:LHG:C35	2.94	0.43
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.55	0.43
23:B:612:CLA:HMB2	23:B:613:CLA:C2B	4.08	0.43
4:D:24:ARG:NH1	41:D:643:HOH:O	2.51	0.43
36:D:410:LHG:H332	36:D:410:LHG:H132	2.01	0.43
10:K:46:ARG:NH1	41:K:207:HOH:O	2.50	0.43
19:Z:46:LEU:O	19:Z:49:ALA:HB3	2.76	0.43
27:B:622:LMG:H332	11:L:35:PHE:CE2	2.53	0.43
28:A:414:PL9:H512	26:D:407:SQD:H301	1.98	0.43
5:E:8:ARG:HA	5:E:9:PRO:HD3	2.17	0.43
11:L:24[A]:ILE:HD11	12:M:18:PRO:HB2	1.98	0.43
13:O:180:GLU:CD	13:O:180:GLU:H	2.22	0.43
23:C:501:CLA:C4D	23:C:503:CLA:H2	2.48	0.43
23:D:403:CLA:HBB1	23:D:403:CLA:CMB	2.61	0.43
3:C:275:SER:HB3	23:C:509:CLA:HED3	1.99	0.43
23:D:403:CLA:CBB	23:D:403:CLA:HMB1	2.63	0.43
13:O:39:ARG:HG2	13:O:246:ALA:HB2	2.01	0.43
1:A:121[B]:LEU:HG	27:A:413:LMG:H181	2.00	0.43
23:B:609:CLA:H161	23:B:609:CLA:H141	1.91	0.43
23:B:616:CLA:OBD	23:B:617:CLA:HHC	5.99	0.43
19:Z:31:GLN:O	19:Z:33:TRP:N	2.52	0.43
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	2.35	0.43
11:L:7:ARG:HH12	29:L:102:UNL:C4	2.32	0.43
25:T:101:BCR:C38	25:T:101:BCR:C23	2.99	0.43
17:Y:26:ALA:O	17:Y:30:ILE:HB	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:214:MET:CE	1:A:255:PHE:CE1	4.93	0.43
1:A:249:VAL:HG12	2:B:491:VAL:HG21	2.01	0.43
2:B:156:PHE:HB3	2:B:162:PHE:HB3	2.30	0.43
23:D:403:CLA:H162	7:H:33:VAL:HG13	10.84	0.43
25:K:101:BCR:C23	25:K:101:BCR:H382	2.62	0.43
2:B:462:PHE:CZ	23:B:614:CLA:HMB3	2.53	0.43
23:B:607:CLA:HMB1	23:B:607:CLA:HBB1	2.01	0.43
19:Z:8:ALA:O	19:Z:11:ALA:HB3	2.48	0.43
1:A:259:ILE:HD12	28:A:414:PL9:H251	2.00	0.42
2:B:61:PHE:CE1	23:B:610:CLA:HMB3	26.36	0.42
12:M:3:VAL:HG11	14:T:2:GLU:HG2	2.01	0.42
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.14	0.42
23:B:604:CLA:C4D	23:B:606:CLA:H43	2.49	0.42
1:A:331:MET:SD	4:D:347:PRO:HB2	2.73	0.42
23:C:510:CLA:HBB1	23:C:510:CLA:HMB1	1.99	0.42
1:A:248[A]:ILE:CD1	4:D:237:PRO:O	2.67	0.42
1:A:215:HIS:ND1	28:A:414:PL9:O1	2.42	0.42
25:B:619:BCR:H363	25:T:101:BCR:H19C	35.17	0.42
23:C:501:CLA:H192	23:C:506:CLA:C1B	2.49	0.42
25:T:101:BCR:HC7	25:T:101:BCR:H331	1.75	0.42
26:D:407:SQD:H241	18:X:31:ILE:HD13	2.01	0.42
3:C:179:ALA:O	3:C:184:GLY:HA2	2.30	0.42
3:C:390:ARG:HD3	16:V:90:GLU:O	2.19	0.42
3:C:302:TYR:O	3:C:422:PRO:HD2	2.59	0.42
5:E:8:ARG:HH21	5:E:12:ASP:HB3	2.98	0.42
12:M:28:GLN:O	12:M:32:GLN:HG3	2.19	0.42
25:D:404:BCR:C38	27:D:411:LMG:H231	2.50	0.42
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.00	0.42
25:A:411:BCR:C8	25:A:411:BCR:H331	2.48	0.42
26:A:412:SQD:H271	36:D:410:LHG:H162	2.01	0.42
2:B:493:TRP:HD1	5:E:5:THR:CG2	2.32	0.42
23:B:612:CLA:HMB1	23:B:612:CLA:CBB	2.41	0.42
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.02	0.42
4:D:61:HIS:HB3	4:D:63:LEU:HG	2.19	0.42
1:A:12:ASN:O	1:A:16:ARG:HG3	2.48	0.42
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.51	0.42
4:D:209:LEU:HD23	4:D:209:LEU:C	2.40	0.42
1:A:334:ARG:HD3	4:D:320:LEU:HD13	2.08	0.42
2:B:270:PRO:HG2	2:B:317:ASN:O	2.36	0.41
3:C:279:LEU:HA	3:C:282:MET:HE3	2.34	0.41
4:D:61:HIS:CE1	4:D:168:PHE:CE2	3.08	0.41
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:D:404:BCR:H11C	25:D:404:BCR:H341	1.99	0.41
5:E:14:ILE:HD12	9:J:13:VAL:HG11	2.09	0.41
3:C:471:SER:HB3	3:C:473:ASP:OXT	2.19	0.41
2:B:90:PHE:CE1	23:B:609:CLA:H162	46.96	0.41
4:D:192:THR:HG23	23:D:402:CLA:HBC2	2.25	0.41
5:E:13:ILE:HG21	37:F:101:HEM:HAD2	2.08	0.41
13:O:20:PRO:HB2	13:O:240:TYR:CD1	2.56	0.41
2:B:498:LYS:HA	4:D:24:ARG:HA	2.23	0.41
23:B:606:CLA:H41	23:B:606:CLA:H62	1.80	0.41
23:B:617:CLA:H61	23:B:617:CLA:H41	1.76	0.41
23:C:506:CLA:HMB2	23:C:507:CLA:NB	2.36	0.41
3:C:95:LEU:HD21	23:C:501:CLA:OBD	2.21	0.41
2:B:103:LEU:HD21	23:B:608:CLA:HMC3	16.02	0.41
36:D:409:LHG:H242	36:D:409:LHG:H272	4.29	0.41
16:V:122:GLU:HG3	16:V:126:LEU:HD12	2.22	0.41
2:B:349:LYS:HE2	2:B:349:LYS:HB3	1.91	0.41
23:B:615:CLA:H161	27:B:622:LMG:C43	2.51	0.41
3:C:377:LEU:HG	3:C:381:LYS:HE2	2.02	0.41
23:B:617:CLA:H43	23:B:617:CLA:H11	4.62	0.41
3:C:276:LEU:HD21	23:C:508:CLA:CAB	2.51	0.41
25:D:404:BCR:H361	25:D:404:BCR:H20C	1.86	0.41
3:C:390:ARG:HD3	16:V:100:ILE:HD12	2.11	0.41
25:A:411:BCR:H351	25:A:411:BCR:H15C	1.93	0.41
2:B:278:SER:HB3	2:B:281:GLN:HE21	1.86	0.41
25:K:101:BCR:C23	25:K:101:BCR:C38	3.11	0.41
23:B:605:CLA:H161	23:B:605:CLA:H141	1.89	0.41
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.21	0.41
3:C:173:LEU:HD23	3:C:173:LEU:HA	2.21	0.41
37:F:101:HEM:CMB	37:F:101:HEM:HBB2	2.57	0.41
4:D:296:TYR:CE2	4:D:319:LEU:HD22	2.81	0.41
13:O:133:VAL:O	13:O:133:VAL:HG12	2.30	0.41
14:T:29:ILE:O	14:T:30:THR:CB	3.22	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	2.02	0.40
13:O:33:ASP:OD1	13:O:35:SER:CB	3.29	0.40
18:X:15[A]:LEU:HA	18:X:15[A]:LEU:HD23	1.85	0.40
17:Y:27:MET:HE2	17:Y:27:MET:HB3	1.97	0.40
3:C:213:LEU:HD11	25:C:515:BCR:C20	2.52	0.40
3:C:78:GLU:CD	16:V:106[A]:ASN:HD21	2.21	0.40
26:D:407:SQD:H321	18:X:24:THR:HA	2.03	0.40
1:A:339:PHE:HB3	1:A:340:PRO:HD2	2.03	0.40
2:B:159:THR:O	2:B:180:PRO:HB3	2.22	0.40
2:B:262:THR:C	2:B:264:PRO:HD3	2.42	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:L:101:LHG:H142	36:L:101:LHG:H171	1.93	0.40
16:V:123:PRO:HD3	16:V:130:TRP:CD1	2.69	0.40
1:A:246:TYR:CE2	1:A:248[A]:ILE:HG22	2.56	0.40
2:B:71:VAL:HG21	2:B:96:VAL:HG21	2.03	0.40
25:C:515:BCR:C33	25:C:515:BCR:C8	2.97	0.40
25:K:102:BCR:H371	25:K:102:BCR:H24C	1.88	0.40
15:U:68:THR:O	15:U:72:LYS:HG3	2.21	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	Distance(Å)	Clash(Å)
41:O:479[B]:HOH:O	41:c:1167:HOH:O[2_455]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	50	37
1	a	336/344 (98%)	329 (98%)	7 (2%)	0	100	100
2	B	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
2	b	508/504 (101%)	497 (98%)	11 (2%)	0	100	100
3	C	452/455 (99%)	442 (98%)	9 (2%)	1 (0%)	56	44
3	c	457/455 (100%)	442 (97%)	13 (3%)	2 (0%)	43	29
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
7	h	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	14	3
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	3	0
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	37/40 (92%)	35 (95%)	2 (5%)	0	100	100
10	K	36/37 (97%)	36 (100%)	0	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	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	247/244 (101%)	238 (96%)	8 (3%)	1 (0%)	43	29
13	o	242/244 (99%)	232 (96%)	9 (4%)	1 (0%)	43	29
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	129 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	2 (3%)	3 (5%)	3	0
19	z	58/62 (94%)	50 (86%)	5 (9%)	3 (5%)	3	0
All	All	5224/5344 (98%)	5075 (97%)	134 (3%)	15 (0%)	50	37

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
19	Z	31	GLN

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Mol	Chain	Res	Type
19	Z	32	ASP
8	i	36	ASP
19	z	31	GLN
3	C	416	SER
19	Z	2	THR
3	c	416[A]	SER
3	c	416[B]	SER
19	z	3	ILE
19	z	32	ASP
8	i	34	ARG
13	o	34	SER
7	h	63	LYS
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	272/279 (98%)	267 (98%)	5 (2%)	71	66
1	a	271/279 (97%)	269 (99%)	2 (1%)	91	90
2	B	407/402 (101%)	404 (99%)	3 (1%)	91	90
2	b	399/402 (99%)	393 (98%)	6 (2%)	76	73
3	C	355/356 (100%)	347 (98%)	8 (2%)	63	55
3	c	358/356 (101%)	349 (98%)	9 (2%)	60	50
4	D	275/276 (100%)	273 (99%)	2 (1%)	91	90
4	d	278/276 (101%)	274 (99%)	4 (1%)	78	75
5	E	71/72 (99%)	70 (99%)	1 (1%)	78	75
5	e	68/72 (94%)	66 (97%)	2 (3%)	55	44
6	F	27/38 (71%)	26 (96%)	1 (4%)	45	32
6	f	26/38 (68%)	25 (96%)	1 (4%)	44	31
7	H	53/53 (100%)	52 (98%)	1 (2%)	69	63
7	h	53/53 (100%)	52 (98%)	1 (2%)	69	63
8	I	31/34 (91%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	33/34 (97%)	32 (97%)	1 (3%)	53	42
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	29/30 (97%)	29 (100%)	0	100	100
10	k	28/30 (93%)	27 (96%)	1 (4%)	47	33
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	207/207 (100%)	203 (98%)	4 (2%)	69	63
13	o	206/207 (100%)	203 (98%)	3 (2%)	76	73
14	T	25/28 (89%)	24 (96%)	1 (4%)	42	29
14	t	25/28 (89%)	24 (96%)	1 (4%)	42	29
15	U	83/89 (93%)	81 (98%)	2 (2%)	61	53
15	u	83/89 (93%)	83 (100%)	0	100	100
16	V	116/117 (99%)	116 (100%)	0	100	100
16	v	115/117 (98%)	114 (99%)	1 (1%)	87	86
17	Y	19/23 (83%)	18 (95%)	1 (5%)	32	18
17	y	18/23 (78%)	16 (89%)	2 (11%)	9	3
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	30/33 (91%)	29 (97%)	1 (3%)	50	37
19	Z	47/52 (90%)	46 (98%)	1 (2%)	66	59
19	z	40/52 (77%)	38 (95%)	2 (5%)	34	20
All	All	4253/4368 (97%)	4186 (98%)	67 (2%)	76	70

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	PRO
1	A	229	GLU
1	A	244	GLU
1	A	248[A]	ILE
1	A	248[B]	ILE
2	B	53	ASN

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Mol	Chain	Res	Type
2	B	467	ILE
2	B	472	ARG
3	C	104	GLU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	391[A]	ARG
3	C	391[B]	ARG
3	C	418	ASN
3	C	471	SER
4	D	90	LEU
4	D	180	ARG
5	E	4	THR
6	F	44	GLN
7	H	49	TYR
13	O	59	LYS
13	O	110	MET
13	O	118	LEU
13	O	207	ARG
14	T	2	GLU
15	U	24	LYS
15	U	70	ARG
17	Y	27	MET
19	Z	6	GLN
1	a	244	GLU
1	a	261	GLN
2	b	246	PHE
2	b	362	PHE
2	b	373	LYS
2	b	472	ARG
2	b	476	ARG
2	b	479	PHE
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	355	THR
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	416[A]	SER
3	c	416[B]	SER
3	c	418	ASN
4	d	24	ARG

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Mol	Chain	Res	Type
4	d	150	ILE
4	d	180	ARG
4	d	329	MET
5	e	60	GLN
5	e	62	SER
6	f	15	ILE
7	h	49	TYR
8	i	38	GLU
10	k	27	VAL
13	o	54	GLU
13	o	64	GLU
13	o	118	LEU
14	t	2	GLU
16	v	23	GLU
17	y	30	ILE
17	y	41	VAL
18	x	39	ARG
19	z	3	ILE
19	z	29	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
2	B	53	ASN
2	B	281	GLN
2	B	331	ASN
2	B	497	GLN
3	C	311	GLN
11	L	6	ASN
13	O	82	GLN
13	O	104	GLN
16	V	34	GLN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	281	GLN
2	b	331	ASN
2	b	338	GLN
3	c	311	GLN
4	d	332	GLN
13	o	36	GLN

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Mol	Chain	Res	Type
13	o	82	GLN
13	o	104	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

10 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	HSK	D	336[A]	-	6,7,12	0.67	0	7,8,16	6.09	4 (57%)
4	HSK	D	336[B]	-	7,8,12	1.96	2 (28%)	7,10,16	4.11	4 (57%)
8	FME	I	1	8	9,9,10	5.84	1 (11%)	6,9,11	0.92	0
12	FME	M	1	12	9,9,10	5.49	1 (11%)	6,9,11	1.65	2 (33%)
14	FME	T	1	14	9,9,10	5.81	2 (22%)	6,9,11	0.99	0
4	HSK	d	336[A]	-	6,7,12	0.61	0	7,8,16	4.95	1 (14%)
4	HSK	d	336[B]	-	7,8,12	1.67	2 (28%)	7,10,16	4.15	5 (71%)
8	FME	i	1	8	9,9,10	5.70	1 (11%)	6,9,11	1.14	0
12	FME	m	1	12	9,9,10	6.23	1 (11%)	6,9,11	1.82	2 (33%)
14	FME	t	1	14	9,9,10	6.91	2 (22%)	6,9,11	1.14	0

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	HSK	D	336[A]	-	-	0/1/2/8	0/1/1/1
4	HSK	D	336[B]	-	-	0/0/2/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/7/9/11	0/0/0/0
12	FME	M	1	12	-	0/7/9/11	0/0/0/0
14	FME	T	1	14	-	0/7/9/11	0/0/0/0
4	HSK	d	336[A]	-	-	0/1/2/8	0/1/1/1
4	HSK	d	336[B]	-	-	0/0/2/8	0/1/1/1
8	FME	i	1	8	-	0/7/9/11	0/0/0/0
12	FME	m	1	12	-	0/7/9/11	0/0/0/0
14	FME	t	1	14	-	0/7/9/11	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	O-C	20.48	1.25	1.11
12	m	1	FME	O-C	18.50	1.24	1.11
8	I	1	FME	O-C	17.38	1.23	1.11
14	T	1	FME	O-C	17.20	1.23	1.11
8	i	1	FME	O-C	17.08	1.23	1.11
12	M	1	FME	O-C	16.33	1.22	1.11
4	D	336[B]	HSK	OM-ND1	4.37	1.47	1.37
4	d	336[B]	HSK	OM-ND1	3.63	1.45	1.37
14	T	1	FME	CA-C	2.67	1.54	1.49
14	t	1	FME	CA-C	2.57	1.54	1.49
4	D	336[B]	HSK	CE1-ND1	-2.38	1.32	1.36
4	d	336[B]	HSK	CE1-ND1	-2.18	1.33	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	336[A]	HSK	NE2-CE1-ND1	-15.47	107.44	115.81
4	d	336[A]	HSK	NE2-CE1-ND1	-12.53	109.03	115.81
4	D	336[B]	HSK	NE2-CE1-ND1	-8.35	105.50	112.86
4	d	336[B]	HSK	NE2-CE1-ND1	-8.31	105.53	112.86
4	d	336[B]	HSK	CE1-ND1-CG	5.72	112.71	105.28
4	D	336[B]	HSK	CE1-ND1-CG	5.54	112.47	105.28
12	M	1	FME	CE-SD-CG	2.84	110.49	100.38
12	M	1	FME	CG-CB-CA	2.63	120.80	112.98
12	m	1	FME	CG-CB-CA	2.59	120.69	112.98
4	D	336[B]	HSK	CD2-NE2-CE1	2.49	109.62	105.79
4	d	336[B]	HSK	CD2-NE2-CE1	2.47	109.58	105.79
4	D	336[A]	HSK	CD2-NE2-CE1	2.46	109.58	105.79
12	m	1	FME	CE-SD-CG	2.38	108.84	100.38
4	d	336[B]	HSK	CD2-CG-ND1	-2.35	104.96	108.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	336[B]	HSK	CB-CG-CD2	-2.22	126.60	130.54
4	d	336[B]	HSK	CB-CG-CD2	-2.12	126.77	130.54
4	D	336[A]	HSK	CE1-ND1-CG	2.06	108.82	104.93
4	D	336[A]	HSK	CB-CG-ND1	2.01	125.67	122.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 276 ligands modelled in this entry, 43 are unknown and 15 are monoatomic - leaving 218 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	401	1,3,41	8,15,15	12.19	8 (100%)	0,32,32	0.00	-
23	CLA	A	405	-	73,73,73	1.84	16 (21%)	96,113,113	2.38	35 (36%)
23	CLA	A	406	41	73,73,73	2.08	20 (27%)	96,113,113	2.64	42 (43%)
23	CLA	A	407	41	73,73,73	2.06	16 (21%)	96,113,113	2.54	35 (36%)
24	PHO	A	408	-	69,69,69	3.18	11 (15%)	92,99,99	2.35	30 (32%)
24	PHO	A	409	-	69,69,69	3.12	15 (21%)	92,99,99	2.40	26 (28%)
23	CLA	A	410	-	73,73,73	1.90	20 (27%)	96,113,113	2.73	33 (34%)
25	BCR	A	411	-	41,41,41	1.00	0	56,56,56	1.47	11 (19%)
26	SQD	A	412	-	54,54,54	1.36	3 (5%)	65,65,65	2.52	18 (27%)
27	LMG	A	413	-	51,51,55	2.17	4 (7%)	59,59,63	1.31	4 (6%)
28	PL9	A	414	-	55,55,55	0.97	3 (5%)	69,69,69	1.56	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	A	418	-	54,54,54	1.35	3 (5%)	65,65,65	1.85	13 (20%)
30	LMT	A	419	-	36,36,36	0.81	1 (2%)	47,47,47	1.39	5 (10%)
31	GOL	A	421	-	5,5,5	0.81	0	5,5,5	0.54	0
31	GOL	A	422	-	5,5,5	0.37	0	5,5,5	0.56	0
31	GOL	A	423	32	5,5,5	0.33	0	5,5,5	0.75	0
23	CLA	B	602	41	73,73,73	2.29	23 (31%)	96,113,113	2.54	32 (33%)
23	CLA	B	603	-	73,73,73	2.29	21 (28%)	96,113,113	2.08	30 (31%)
23	CLA	B	604	-	73,73,73	1.99	20 (27%)	96,113,113	2.82	36 (37%)
23	CLA	B	605	-	73,73,73	1.86	18 (24%)	96,113,113	2.24	31 (32%)
23	CLA	B	606	-	73,73,73	1.93	14 (19%)	96,113,113	2.40	31 (32%)
23	CLA	B	607	-	73,73,73	2.09	14 (19%)	96,113,113	2.57	31 (32%)
23	CLA	B	608	41	73,73,73	2.06	19 (26%)	96,113,113	2.46	30 (31%)
23	CLA	B	609	-	73,73,73	1.75	14 (19%)	96,113,113	2.76	32 (33%)
23	CLA	B	610	-	73,73,73	1.97	18 (24%)	96,113,113	2.37	29 (30%)
23	CLA	B	611	41	73,73,73	2.02	20 (27%)	96,113,113	2.54	34 (35%)
23	CLA	B	612	-	73,73,73	1.90	17 (23%)	96,113,113	2.68	34 (35%)
23	CLA	B	613	-	73,73,73	2.00	19 (26%)	96,113,113	2.22	35 (36%)
23	CLA	B	614	-	73,73,73	1.81	17 (23%)	96,113,113	2.35	31 (32%)
23	CLA	B	615	-	73,73,73	2.07	14 (19%)	96,113,113	2.40	30 (31%)
23	CLA	B	616	-	73,73,73	2.14	18 (24%)	96,113,113	2.28	29 (30%)
23	CLA	B	617	-	73,73,73	1.86	20 (27%)	96,113,113	2.47	31 (32%)
25	BCR	B	618	-	41,41,41	1.10	2 (4%)	56,56,56	1.55	10 (17%)
25	BCR	B	619	-	41,41,41	1.16	3 (7%)	56,56,56	1.20	5 (8%)
25	BCR	B	620	-	41,41,41	0.98	1 (2%)	56,56,56	1.62	10 (17%)
26	SQD	B	621	-	54,54,54	1.33	5 (9%)	65,65,65	2.17	15 (23%)
27	LMG	B	622	-	51,51,55	2.15	4 (7%)	59,59,63	1.62	10 (16%)
30	LMT	B	623	-	36,36,36	0.97	2 (5%)	47,47,47	1.44	8 (17%)
33	HTG	B	624	-	19,19,19	1.07	1 (5%)	24,24,24	1.81	6 (25%)
33	HTG	B	625	-	19,19,19	0.95	2 (10%)	24,24,24	1.71	5 (20%)
33	HTG	B	626	-	19,19,19	0.87	1 (5%)	24,24,24	2.08	2 (8%)
33	HTG	B	630	-	19,19,19	1.00	2 (10%)	24,24,24	1.74	2 (8%)
33	HTG	B	631	-	19,19,19	0.80	2 (10%)	24,24,24	2.23	3 (12%)
31	GOL	B	633	-	5,5,5	0.34	0	5,5,5	1.43	1 (20%)
31	GOL	B	634	-	5,5,5	0.79	0	5,5,5	0.69	0
31	GOL	B	635	-	5,5,5	0.51	0	5,5,5	1.00	0
31	GOL	B	636	-	5,5,5	0.40	0	5,5,5	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GOL	B	637	-	5,5,5	0.47	0	5,5,5	1.13	1 (20%)
31	GOL	B	638	-	5,5,5	0.43	0	5,5,5	0.84	0
23	CLA	C	501	-	73,73,73	2.05	22 (30%)	96,113,113	2.51	27 (28%)
23	CLA	C	502	-	73,73,73	1.87	16 (21%)	96,113,113	2.62	35 (36%)
23	CLA	C	503	-	73,73,73	2.16	21 (28%)	96,113,113	2.30	26 (27%)
23	CLA	C	504	41	73,73,73	2.09	17 (23%)	96,113,113	2.25	31 (32%)
23	CLA	C	505	-	73,73,73	2.05	19 (26%)	96,113,113	2.27	31 (32%)
23	CLA	C	506	-	73,73,73	2.12	17 (23%)	96,113,113	2.36	31 (32%)
23	CLA	C	507	41	73,73,73	2.21	19 (26%)	96,113,113	2.28	24 (25%)
23	CLA	C	508	-	73,73,73	2.32	22 (30%)	96,113,113	2.04	26 (27%)
23	CLA	C	509	-	73,73,73	2.04	19 (26%)	96,113,113	2.28	30 (31%)
23	CLA	C	510	-	73,73,73	1.99	19 (26%)	96,113,113	2.54	33 (34%)
23	CLA	C	511	3	73,73,73	2.20	21 (28%)	96,113,113	2.35	27 (28%)
23	CLA	C	512	-	73,73,73	2.24	19 (26%)	96,113,113	2.24	29 (30%)
23	CLA	C	513	-	73,73,73	2.43	20 (27%)	96,113,113	2.10	27 (28%)
25	BCR	C	514	-	41,41,41	0.86	0	56,56,56	1.29	8 (14%)
25	BCR	C	515	-	41,41,41	0.90	1 (2%)	56,56,56	1.44	4 (7%)
34	DGD	C	516	-	63,63,67	1.72	5 (7%)	77,77,81	1.42	14 (18%)
34	DGD	C	517	-	63,63,67	1.26	3 (4%)	77,77,81	1.13	6 (7%)
34	DGD	C	518	-	63,63,67	1.13	5 (7%)	77,77,81	1.32	9 (11%)
27	LMG	C	519	-	51,51,55	1.88	5 (9%)	59,59,63	1.49	9 (15%)
30	LMT	C	520	-	36,36,36	0.60	1 (2%)	47,47,47	1.54	8 (17%)
33	HTG	C	521	-	19,19,19	0.85	1 (5%)	24,24,24	1.62	1 (4%)
33	HTG	C	522	-	19,19,19	0.95	2 (10%)	24,24,24	2.41	3 (12%)
31	GOL	C	524	-	5,5,5	0.32	0	5,5,5	1.71	1 (20%)
31	GOL	C	525	-	5,5,5	0.75	0	5,5,5	0.86	0
31	GOL	C	526	-	5,5,5	0.62	0	5,5,5	0.48	0
35	BCT	D	401	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	D	402	-	73,73,73	2.26	21 (28%)	96,113,113	2.68	42 (43%)
23	CLA	D	403	-	73,73,73	2.13	23 (31%)	96,113,113	2.25	33 (34%)
25	BCR	D	404	-	41,41,41	1.14	3 (7%)	56,56,56	2.02	19 (33%)
28	PL9	D	405	-	55,55,55	1.34	10 (18%)	69,69,69	1.66	15 (21%)
34	DGD	D	406	-	52,53,67	1.28	5 (9%)	59,61,81	1.43	8 (13%)
26	SQD	D	407	-	45,45,54	1.51	6 (13%)	56,56,65	2.43	17 (30%)
36	LHG	D	408	-	48,48,48	0.77	1 (2%)	54,54,54	1.44	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LHG	D	409	-	48,48,48	0.80	2 (4%)	54,54,54	1.08	5 (9%)
36	LHG	D	410	-	45,45,48	1.43	4 (8%)	51,51,54	1.03	3 (5%)
27	LMG	D	411	39	51,51,55	1.45	4 (7%)	59,59,63	1.04	3 (5%)
33	HTG	D	414	-	19,19,19	0.99	1 (5%)	24,24,24	1.64	2 (8%)
31	GOL	D	415	-	5,5,5	0.66	0	5,5,5	1.21	0
36	LHG	E	101	-	48,48,48	0.97	2 (4%)	54,54,54	1.01	4 (7%)
37	HEM	F	101	5,6	42,50,50	3.58	14 (33%)	27,82,82	2.39	8 (29%)
30	LMT	F	102	-	36,36,36	0.73	1 (2%)	47,47,47	1.19	3 (6%)
38	RRX	H	101	-	42,42,42	1.07	3 (7%)	58,58,58	1.56	11 (18%)
34	DGD	H	102	-	63,63,67	1.36	4 (6%)	77,77,81	1.41	13 (16%)
30	LMT	J	102	-	24,24,36	0.81	1 (4%)	29,29,47	1.26	4 (13%)
25	BCR	K	101	-	41,41,41	0.86	0	56,56,56	1.65	12 (21%)
25	BCR	K	102	-	41,41,41	0.92	1 (2%)	56,56,56	1.66	11 (19%)
36	LHG	L	101	-	48,48,48	0.78	2 (4%)	54,54,54	1.49	8 (14%)
26	SQD	L	103	-	54,54,54	1.28	4 (7%)	65,65,65	2.05	14 (21%)
31	GOL	L	104	-	5,5,5	0.46	0	5,5,5	0.63	0
30	LMT	M	101	-	36,36,36	0.84	1 (2%)	47,47,47	1.30	6 (12%)
30	LMT	M	102	-	36,36,36	0.62	0	47,47,47	1.35	8 (17%)
40	SO4	O	302	-	4,4,4	0.68	0	6,6,6	0.35	0
33	HTG	O	303	-	19,19,19	1.16	2 (10%)	24,24,24	1.54	2 (8%)
31	GOL	O	304	-	5,5,5	0.49	0	5,5,5	0.63	0
25	BCR	T	101	-	41,41,41	0.86	0	56,56,56	1.62	12 (21%)
33	HTG	U	201	-	7,8,19	1.42	1 (14%)	6,7,24	0.79	0
37	HEM	V	201	16	42,50,50	3.75	16 (38%)	27,82,82	1.65	5 (18%)
33	HTG	V	202	-	12,13,19	0.80	1 (8%)	17,18,24	3.35	7 (41%)
31	GOL	V	203	-	5,5,5	0.94	0	5,5,5	0.84	0
31	GOL	V	204	-	5,5,5	0.29	0	5,5,5	0.37	0
31	GOL	V	205	-	5,5,5	0.58	0	5,5,5	0.36	0
27	LMG	Z	101	-	51,51,55	1.63	5 (9%)	59,59,63	1.38	7 (11%)
30	LMT	Z	102	-	36,36,36	0.65	1 (2%)	47,47,47	0.92	0
26	SQD	a	401	-	54,54,54	1.46	3 (5%)	65,65,65	1.75	10 (15%)
30	LMT	a	402	-	36,36,36	0.74	1 (2%)	47,47,47	1.65	10 (21%)
20	OEX	a	404	1,3,41	8,15,15	10.55	7 (87%)	0,32,32	0.00	-
35	BCT	a	408	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	a	409	-	73,73,73	1.92	17 (23%)	96,113,113	2.40	32 (33%)
23	CLA	a	410	41	73,73,73	1.86	17 (23%)	96,113,113	2.50	29 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	411	41	73,73,73	1.83	21 (28%)	96,113,113	2.53	41 (42%)
24	PHO	a	412	-	69,69,69	3.59	12 (17%)	92,99,99	2.13	27 (29%)
24	PHO	a	413	-	69,69,69	3.20	17 (24%)	92,99,99	2.25	29 (31%)
23	CLA	a	414	-	73,73,73	1.94	17 (23%)	96,113,113	2.71	40 (41%)
25	BCR	a	415	-	41,41,41	1.19	3 (7%)	56,56,56	1.43	8 (14%)
26	SQD	a	416	-	54,54,54	1.32	3 (5%)	65,65,65	2.59	17 (26%)
36	LHG	a	417	-	39,39,48	1.35	3 (7%)	45,45,54	0.98	3 (6%)
27	LMG	a	418	-	51,51,55	2.02	4 (7%)	59,59,63	1.36	4 (6%)
28	PL9	a	419	-	55,55,55	0.90	3 (5%)	69,69,69	1.91	20 (28%)
31	GOL	a	422	-	5,5,5	0.62	0	5,5,5	0.78	0
31	GOL	a	423	-	5,5,5	0.56	0	5,5,5	0.51	0
31	GOL	a	424	-	5,5,5	0.58	0	5,5,5	0.79	0
33	HTG	b	601	-	19,19,19	0.91	2 (10%)	24,24,24	1.36	2 (8%)
33	HTG	b	602	-	19,19,19	0.74	0	24,24,24	1.37	3 (12%)
23	CLA	b	604	41	73,73,73	2.32	21 (28%)	96,113,113	2.26	26 (27%)
23	CLA	b	605	-	73,73,73	2.17	20 (27%)	96,113,113	2.37	33 (34%)
23	CLA	b	606	-	73,73,73	1.96	17 (23%)	96,113,113	2.75	37 (38%)
23	CLA	b	607	-	73,73,73	2.00	18 (24%)	96,113,113	2.36	31 (32%)
23	CLA	b	608	-	73,73,73	1.93	13 (17%)	96,113,113	2.48	34 (35%)
23	CLA	b	609	-	73,73,73	2.25	23 (31%)	96,113,113	2.28	33 (34%)
23	CLA	b	610	41	73,73,73	2.24	21 (28%)	96,113,113	2.17	30 (31%)
23	CLA	b	611	-	73,73,73	2.06	16 (21%)	96,113,113	2.21	24 (25%)
23	CLA	b	612	-	73,73,73	2.32	21 (28%)	96,113,113	2.11	30 (31%)
23	CLA	b	613	41	73,73,73	2.02	19 (26%)	96,113,113	2.38	25 (26%)
23	CLA	b	614	-	73,73,73	1.99	17 (23%)	96,113,113	2.25	30 (31%)
23	CLA	b	615	-	73,73,73	2.09	14 (19%)	96,113,113	2.42	30 (31%)
23	CLA	b	616	-	73,73,73	2.05	15 (20%)	96,113,113	2.44	34 (35%)
23	CLA	b	617	-	73,73,73	1.71	15 (20%)	96,113,113	2.59	37 (38%)
23	CLA	b	618	-	73,73,73	2.15	17 (23%)	96,113,113	2.63	36 (37%)
23	CLA	b	619	-	73,73,73	2.04	20 (27%)	96,113,113	2.54	32 (33%)
25	BCR	b	620	-	41,41,41	1.03	2 (4%)	56,56,56	1.71	14 (25%)
25	BCR	b	621	-	41,41,41	1.14	3 (7%)	56,56,56	1.27	7 (12%)
25	BCR	b	622	-	41,41,41	0.95	1 (2%)	56,56,56	1.25	5 (8%)
27	LMG	b	623	-	51,51,55	1.73	4 (7%)	59,59,63	1.46	7 (11%)
30	LMT	b	624	-	24,25,36	0.71	1 (4%)	29,30,47	1.44	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMT	b	625	-	24,24,36	0.55	0	29,29,47	1.31	4 (13%)
33	HTG	b	626	-	19,19,19	0.99	1 (5%)	24,24,24	1.64	5 (20%)
33	HTG	b	627	-	19,19,19	1.05	2 (10%)	24,24,24	1.88	1 (4%)
31	GOL	b	632	-	5,5,5	0.50	0	5,5,5	1.37	1 (20%)
31	GOL	b	633	-	5,5,5	0.34	0	5,5,5	0.86	0
31	GOL	b	634	-	5,5,5	0.44	0	5,5,5	0.23	0
31	GOL	b	635	-	5,5,5	0.74	0	5,5,5	0.96	0
31	GOL	b	636	-	5,5,5	0.50	0	5,5,5	0.93	0
23	CLA	c	902	-	73,73,73	2.04	20 (27%)	96,113,113	2.53	31 (32%)
23	CLA	c	903	-	73,73,73	2.15	21 (28%)	96,113,113	2.55	32 (33%)
23	CLA	c	904	-	73,73,73	2.25	22 (30%)	96,113,113	2.12	28 (29%)
23	CLA	c	905	41	73,73,73	2.29	20 (27%)	96,113,113	2.38	32 (33%)
23	CLA	c	906	-	73,73,73	2.04	20 (27%)	96,113,113	2.31	33 (34%)
23	CLA	c	907	-	73,73,73	2.15	17 (23%)	96,113,113	2.70	35 (36%)
23	CLA	c	908	41	73,73,73	2.13	19 (26%)	96,113,113	2.46	33 (34%)
23	CLA	c	909	-	73,73,73	2.26	23 (31%)	96,113,113	2.21	28 (29%)
23	CLA	c	910	-	73,73,73	2.32	21 (28%)	96,113,113	2.50	39 (40%)
23	CLA	c	911	-	73,73,73	2.04	22 (30%)	96,113,113	2.10	29 (30%)
23	CLA	c	912	3	73,73,73	2.25	19 (26%)	96,113,113	2.32	28 (29%)
23	CLA	c	913	-	73,73,73	2.39	20 (27%)	96,113,113	2.19	28 (29%)
23	CLA	c	914	-	73,73,73	2.48	20 (27%)	96,113,113	2.11	27 (28%)
25	BCR	c	915	-	41,41,41	0.84	1 (2%)	56,56,56	1.23	6 (10%)
25	BCR	c	916	-	41,41,41	0.94	1 (2%)	56,56,56	1.36	7 (12%)
34	DGD	c	917	-	63,63,67	1.15	4 (6%)	77,77,81	1.32	10 (12%)
34	DGD	c	918	-	63,63,67	1.29	6 (9%)	77,77,81	1.29	11 (14%)
34	DGD	c	919	-	63,63,67	1.28	7 (11%)	77,77,81	1.40	11 (14%)
27	LMG	c	920	-	51,51,55	2.09	6 (11%)	59,59,63	1.29	8 (13%)
27	LMG	c	921	-	51,51,55	1.55	5 (9%)	59,59,63	1.27	7 (11%)
30	LMT	c	922	-	36,36,36	0.73	1 (2%)	47,47,47	1.03	4 (8%)
33	HTG	c	923	-	19,19,19	0.94	2 (10%)	24,24,24	2.01	2 (8%)
33	HTG	c	924	-	19,19,19	0.93	1 (5%)	24,24,24	2.52	5 (20%)
31	GOL	c	927	-	5,5,5	0.58	0	5,5,5	0.43	0
31	GOL	c	928	-	5,5,5	0.26	0	5,5,5	0.80	0
31	GOL	c	929	-	5,5,5	0.45	0	5,5,5	0.79	0
31	GOL	c	930	-	5,5,5	0.38	0	5,5,5	0.72	0
33	HTG	d	401	-	19,19,19	1.01	2 (10%)	24,24,24	1.63	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	402	-	73,73,73	1.86	13 (17%)	96,113,113	2.71	36 (37%)
23	CLA	d	403	-	73,73,73	2.05	22 (30%)	96,113,113	2.55	34 (35%)
25	BCR	d	404	-	41,41,41	0.98	3 (7%)	56,56,56	1.78	14 (25%)
28	PL9	d	405	-	55,55,55	1.33	9 (16%)	69,69,69	1.68	13 (18%)
34	DGD	d	406	-	49,50,67	1.40	5 (10%)	56,58,81	1.50	10 (17%)
36	LHG	d	407	-	48,48,48	0.78	2 (4%)	54,54,54	1.40	7 (12%)
36	LHG	d	408	-	48,48,48	0.76	2 (4%)	54,54,54	1.27	7 (12%)
36	LHG	d	409	-	48,48,48	0.89	3 (6%)	54,54,54	1.03	4 (7%)
27	LMG	d	410	39	51,51,55	1.60	5 (9%)	59,59,63	1.17	8 (13%)
37	HEM	f	101	5,6	42,50,50	3.43	13 (30%)	27,82,82	2.21	6 (22%)
26	SQD	f	102	-	29,32,54	1.20	2 (6%)	29,36,65	1.26	4 (13%)
31	GOL	f	104	32	5,5,5	0.48	0	5,5,5	0.42	0
38	RRX	h	101	-	42,42,42	0.94	0	58,58,58	1.26	8 (13%)
34	DGD	h	102	-	63,63,67	1.24	5 (7%)	77,77,81	1.28	8 (10%)
31	GOL	h	103	-	5,5,5	0.31	0	5,5,5	0.31	0
25	BCR	k	101	-	41,41,41	0.84	1 (2%)	56,56,56	1.45	10 (17%)
25	BCR	k	102	-	41,41,41	0.96	2 (4%)	56,56,56	1.30	5 (8%)
36	LHG	l	101	-	48,48,48	0.81	2 (4%)	54,54,54	1.05	5 (9%)
31	GOL	l	102	-	5,5,5	0.44	0	5,5,5	1.09	0
30	LMT	m	101	-	36,36,36	0.73	0	47,47,47	1.42	9 (19%)
30	LMT	m	102	-	36,36,36	0.71	1 (2%)	47,47,47	1.16	3 (6%)
25	BCR	t	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.80	12 (21%)
30	LMT	t	102	-	24,24,36	0.69	0	29,29,47	1.44	4 (13%)
33	HTG	u	201	-	12,13,19	5.53	1 (8%)	9,14,24	2.68	1 (11%)
37	HEM	v	201	16	42,50,50	3.60	17 (40%)	27,82,82	1.62	4 (14%)
31	GOL	v	202	-	5,5,5	0.55	0	5,5,5	0.50	0
31	GOL	v	203	-	5,5,5	0.70	0	5,5,5	0.44	0
31	GOL	v	204	-	5,5,5	0.33	0	5,5,5	0.60	0
30	LMT	z	101	-	31,32,36	1.06	1 (3%)	41,42,47	1.07	3 (7%)

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	401	1,3,41	-	0/0/68/68	0/0/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	405	-	-	0/37/135/135	0/0/9/9
23	CLA	A	406	41	-	0/37/135/135	0/0/9/9
23	CLA	A	407	41	-	0/37/135/135	0/0/9/9
24	PHO	A	408	-	-	0/49/103/103	0/1/6/6
24	PHO	A	409	-	-	0/49/103/103	0/1/6/6
23	CLA	A	410	-	-	0/37/135/135	0/0/9/9
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
26	SQD	A	412	-	-	0/49/69/69	0/1/1/1
27	LMG	A	413	-	-	0/46/66/70	0/1/1/1
28	PL9	A	414	-	-	0/53/73/73	0/1/1/1
26	SQD	A	418	-	-	0/49/69/69	0/1/1/1
30	LMT	A	419	-	-	0/21/61/61	0/2/2/2
31	GOL	A	421	-	-	0/4/4/4	0/0/0/0
31	GOL	A	422	-	-	0/4/4/4	0/0/0/0
31	GOL	A	423	32	-	0/4/4/4	0/0/0/0
23	CLA	B	602	41	-	0/37/135/135	0/0/9/9
23	CLA	B	603	-	-	0/37/135/135	0/0/9/9
23	CLA	B	604	-	-	0/37/135/135	0/0/9/9
23	CLA	B	605	-	-	0/37/135/135	0/0/9/9
23	CLA	B	606	-	-	0/37/135/135	0/0/9/9
23	CLA	B	607	-	-	0/37/135/135	0/0/9/9
23	CLA	B	608	41	-	0/37/135/135	0/0/9/9
23	CLA	B	609	-	-	0/37/135/135	0/0/9/9
23	CLA	B	610	-	-	0/37/135/135	0/0/9/9
23	CLA	B	611	41	-	0/37/135/135	0/0/9/9
23	CLA	B	612	-	-	0/37/135/135	0/0/9/9
23	CLA	B	613	-	-	0/37/135/135	0/0/9/9
23	CLA	B	614	-	-	0/37/135/135	0/0/9/9
23	CLA	B	615	-	-	0/37/135/135	0/0/9/9
23	CLA	B	616	-	-	0/37/135/135	0/0/9/9
23	CLA	B	617	-	-	0/37/135/135	0/0/9/9
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	SQD	B	621	-	-	0/49/69/69	0/1/1/1
27	LMG	B	622	-	-	0/46/66/70	0/1/1/1
30	LMT	B	623	-	-	0/21/61/61	0/2/2/2
33	HTG	B	624	-	-	0/10/30/30	0/1/1/1
33	HTG	B	625	-	-	0/10/30/30	0/1/1/1
33	HTG	B	626	-	-	0/10/30/30	0/1/1/1
33	HTG	B	630	-	-	0/10/30/30	0/1/1/1
33	HTG	B	631	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	B	633	-	-	0/4/4/4	0/0/0/0
31	GOL	B	634	-	-	0/4/4/4	0/0/0/0
31	GOL	B	635	-	-	0/4/4/4	0/0/0/0
31	GOL	B	636	-	-	0/4/4/4	0/0/0/0
31	GOL	B	637	-	-	0/4/4/4	0/0/0/0
31	GOL	B	638	-	-	0/4/4/4	0/0/0/0
23	CLA	C	501	-	-	0/37/135/135	0/0/9/9
23	CLA	C	502	-	-	0/37/135/135	0/0/9/9
23	CLA	C	503	-	-	0/37/135/135	0/0/9/9
23	CLA	C	504	41	-	0/37/135/135	0/0/9/9
23	CLA	C	505	-	-	0/37/135/135	0/0/9/9
23	CLA	C	506	-	-	0/37/135/135	0/0/9/9
23	CLA	C	507	41	-	0/37/135/135	0/0/9/9
23	CLA	C	508	-	-	0/37/135/135	0/0/9/9
23	CLA	C	509	-	-	0/37/135/135	0/0/9/9
23	CLA	C	510	-	-	0/37/135/135	0/0/9/9
23	CLA	C	511	3	-	0/37/135/135	0/0/9/9
23	CLA	C	512	-	-	0/37/135/135	0/0/9/9
23	CLA	C	513	-	-	0/37/135/135	0/0/9/9
25	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
34	DGD	C	516	-	-	0/51/91/95	0/2/2/2
34	DGD	C	517	-	-	0/51/91/95	0/2/2/2
34	DGD	C	518	-	-	0/51/91/95	0/2/2/2
27	LMG	C	519	-	-	0/46/66/70	0/1/1/1
30	LMT	C	520	-	-	0/21/61/61	0/2/2/2
33	HTG	C	521	-	-	0/10/30/30	0/1/1/1
33	HTG	C	522	-	-	0/10/30/30	0/1/1/1
31	GOL	C	524	-	-	0/4/4/4	0/0/0/0
31	GOL	C	525	-	-	0/4/4/4	0/0/0/0
31	GOL	C	526	-	-	0/4/4/4	0/0/0/0
35	BCT	D	401	21	-	0/0/0/0	0/0/0/0
23	CLA	D	402	-	-	0/37/135/135	0/0/9/9
23	CLA	D	403	-	-	0/37/135/135	0/0/9/9
25	BCR	D	404	-	-	0/29/63/63	0/2/2/2
28	PL9	D	405	-	-	0/53/73/73	0/1/1/1
34	DGD	D	406	-	-	0/47/68/95	0/1/1/2
26	SQD	D	407	-	-	0/40/60/69	0/1/1/1
36	LHG	D	408	-	-	0/53/53/53	0/0/0/0
36	LHG	D	409	-	-	0/53/53/53	0/0/0/0
36	LHG	D	410	-	-	0/50/50/53	0/0/0/0
27	LMG	D	411	39	-	0/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	HTG	D	414	-	-	0/10/30/30	0/1/1/1
31	GOL	D	415	-	-	0/4/4/4	0/0/0/0
36	LHG	E	101	-	-	0/53/53/53	0/0/0/0
37	HEM	F	101	5,6	-	0/14/114/114	0/0/8/8
30	LMT	F	102	-	-	0/21/61/61	0/2/2/2
38	RRX	H	101	-	-	0/29/65/65	0/2/2/2
34	DGD	H	102	-	-	0/51/91/95	0/2/2/2
30	LMT	J	102	-	-	0/15/35/61	0/1/1/2
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
25	BCR	K	102	-	-	0/29/63/63	0/2/2/2
36	LHG	L	101	-	-	0/53/53/53	0/0/0/0
26	SQD	L	103	-	-	0/49/69/69	0/1/1/1
31	GOL	L	104	-	-	0/4/4/4	0/0/0/0
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
40	SO4	O	302	-	-	0/0/0/0	0/0/0/0
33	HTG	O	303	-	-	0/10/30/30	0/1/1/1
31	GOL	O	304	-	-	0/4/4/4	0/0/0/0
25	BCR	T	101	-	-	0/29/63/63	0/2/2/2
33	HTG	U	201	-	-	0/6/6/30	0/0/0/1
37	HEM	V	201	16	-	0/14/114/114	0/0/8/8
33	HTG	V	202	-	-	0/4/24/30	0/1/1/1
31	GOL	V	203	-	-	0/4/4/4	0/0/0/0
31	GOL	V	204	-	-	0/4/4/4	0/0/0/0
31	GOL	V	205	-	-	0/4/4/4	0/0/0/0
27	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
30	LMT	Z	102	-	-	0/21/61/61	0/2/2/2
26	SQD	a	401	-	-	0/49/69/69	0/1/1/1
30	LMT	a	402	-	-	0/21/61/61	0/2/2/2
20	OEX	a	404	1,3,41	-	0/0/68/68	0/0/6/6
35	BCT	a	408	21	-	0/0/0/0	0/0/0/0
23	CLA	a	409	-	-	0/37/135/135	0/0/9/9
23	CLA	a	410	41	-	0/37/135/135	0/0/9/9
23	CLA	a	411	41	-	0/37/135/135	0/0/9/9
24	PHO	a	412	-	-	0/49/103/103	0/1/6/6
24	PHO	a	413	-	-	0/49/103/103	0/1/6/6
23	CLA	a	414	-	-	0/37/135/135	0/0/9/9
25	BCR	a	415	-	-	0/29/63/63	0/2/2/2
26	SQD	a	416	-	-	0/49/69/69	0/1/1/1
36	LHG	a	417	-	-	0/44/44/53	0/0/0/0
27	LMG	a	418	-	-	0/46/66/70	0/1/1/1
28	PL9	a	419	-	-	0/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	a	422	-	-	0/4/4/4	0/0/0/0
31	GOL	a	423	-	-	0/4/4/4	0/0/0/0
31	GOL	a	424	-	-	0/4/4/4	0/0/0/0
33	HTG	b	601	-	-	0/10/30/30	0/1/1/1
33	HTG	b	602	-	-	0/10/30/30	0/1/1/1
23	CLA	b	604	41	-	0/37/135/135	0/0/9/9
23	CLA	b	605	-	-	0/37/135/135	0/0/9/9
23	CLA	b	606	-	-	0/37/135/135	0/0/9/9
23	CLA	b	607	-	-	0/37/135/135	0/0/9/9
23	CLA	b	608	-	-	0/37/135/135	0/0/9/9
23	CLA	b	609	-	-	0/37/135/135	0/0/9/9
23	CLA	b	610	41	-	0/37/135/135	0/0/9/9
23	CLA	b	611	-	-	0/37/135/135	0/0/9/9
23	CLA	b	612	-	-	0/37/135/135	0/0/9/9
23	CLA	b	613	41	-	0/37/135/135	0/0/9/9
23	CLA	b	614	-	-	0/37/135/135	0/0/9/9
23	CLA	b	615	-	-	0/37/135/135	0/0/9/9
23	CLA	b	616	-	-	0/37/135/135	0/0/9/9
23	CLA	b	617	-	-	0/37/135/135	0/0/9/9
23	CLA	b	618	-	-	0/37/135/135	0/0/9/9
23	CLA	b	619	-	-	0/37/135/135	0/0/9/9
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
25	BCR	b	621	-	-	0/29/63/63	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
27	LMG	b	623	-	-	0/46/66/70	0/1/1/1
30	LMT	b	624	-	-	0/17/37/61	0/1/1/2
30	LMT	b	625	-	-	0/15/35/61	0/1/1/2
33	HTG	b	626	-	-	0/10/30/30	0/1/1/1
33	HTG	b	627	-	-	0/10/30/30	0/1/1/1
31	GOL	b	632	-	-	0/4/4/4	0/0/0/0
31	GOL	b	633	-	-	0/4/4/4	0/0/0/0
31	GOL	b	634	-	-	0/4/4/4	0/0/0/0
31	GOL	b	635	-	-	0/4/4/4	0/0/0/0
31	GOL	b	636	-	-	0/4/4/4	0/0/0/0
23	CLA	c	902	-	-	0/37/135/135	0/0/9/9
23	CLA	c	903	-	-	0/37/135/135	0/0/9/9
23	CLA	c	904	-	-	0/37/135/135	0/0/9/9
23	CLA	c	905	41	-	0/37/135/135	0/0/9/9
23	CLA	c	906	-	-	0/37/135/135	0/0/9/9
23	CLA	c	907	-	-	0/37/135/135	0/0/9/9
23	CLA	c	908	41	-	0/37/135/135	0/0/9/9
23	CLA	c	909	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	910	-	-	0/37/135/135	0/0/9/9
23	CLA	c	911	-	-	0/37/135/135	0/0/9/9
23	CLA	c	912	3	-	0/37/135/135	0/0/9/9
23	CLA	c	913	-	-	0/37/135/135	0/0/9/9
23	CLA	c	914	-	-	0/37/135/135	0/0/9/9
25	BCR	c	915	-	-	0/29/63/63	0/2/2/2
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
34	DGD	c	917	-	-	0/51/91/95	0/2/2/2
34	DGD	c	918	-	-	0/51/91/95	0/2/2/2
34	DGD	c	919	-	-	0/51/91/95	0/2/2/2
27	LMG	c	920	-	-	0/46/66/70	0/1/1/1
27	LMG	c	921	-	-	0/46/66/70	0/1/1/1
30	LMT	c	922	-	-	0/21/61/61	0/2/2/2
33	HTG	c	923	-	-	0/10/30/30	0/1/1/1
33	HTG	c	924	-	-	0/10/30/30	0/1/1/1
31	GOL	c	927	-	-	0/4/4/4	0/0/0/0
31	GOL	c	928	-	-	0/4/4/4	0/0/0/0
31	GOL	c	929	-	-	0/4/4/4	0/0/0/0
31	GOL	c	930	-	-	0/4/4/4	0/0/0/0
33	HTG	d	401	-	-	0/10/30/30	0/1/1/1
23	CLA	d	402	-	-	0/37/135/135	0/0/9/9
23	CLA	d	403	-	-	0/37/135/135	0/0/9/9
25	BCR	d	404	-	-	0/29/63/63	0/2/2/2
28	PL9	d	405	-	-	0/53/73/73	0/1/1/1
34	DGD	d	406	-	-	0/44/64/95	0/1/1/2
36	LHG	d	407	-	-	0/53/53/53	0/0/0/0
36	LHG	d	408	-	-	0/53/53/53	0/0/0/0
36	LHG	d	409	-	-	0/53/53/53	0/0/0/0
27	LMG	d	410	39	-	0/46/66/70	0/1/1/1
37	HEM	f	101	5,6	-	0/14/114/114	0/0/8/8
26	SQD	f	102	-	-	0/28/33/69	0/0/0/1
31	GOL	f	104	32	-	0/4/4/4	0/0/0/0
38	RRX	h	101	-	-	0/29/65/65	0/2/2/2
34	DGD	h	102	-	-	0/51/91/95	0/2/2/2
31	GOL	h	103	-	-	0/4/4/4	0/0/0/0
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
25	BCR	k	102	-	-	0/29/63/63	0/2/2/2
36	LHG	l	101	-	-	0/53/53/53	0/0/0/0
31	GOL	l	102	-	-	0/4/4/4	0/0/0/0
30	LMT	m	101	-	-	0/21/61/61	0/2/2/2
30	LMT	m	102	-	-	0/21/61/61	0/2/2/2
25	BCR	t	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	t	102	-	-	0/15/35/61	0/1/1/2
33	HTG	u	201	-	-	0/10/14/30	0/0/0/1
37	HEM	v	201	16	-	0/14/114/114	0/0/8/8
31	GOL	v	202	-	-	0/4/4/4	0/0/0/0
31	GOL	v	203	-	-	0/4/4/4	0/0/0/0
31	GOL	v	204	-	-	0/4/4/4	0/0/0/0
30	LMT	z	101	-	-	0/15/55/61	0/2/2/2

All (1686) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	404	OEX	O1-MN1	-22.59	1.80	2.02
24	a	412	PHO	CHD-C4C	21.89	1.50	1.35
33	u	201	HTG	O3-C3	18.96	1.46	1.25
20	A	401	OEX	O3-MN1	-18.80	1.84	2.02
20	A	401	OEX	O1-MN1	-17.13	1.85	2.02
24	A	408	PHO	CHD-C4C	17.04	1.47	1.35
24	a	413	PHO	CHD-C4C	14.55	1.45	1.35
24	a	413	PHO	C1B-CHB	13.85	1.50	1.35
20	A	401	OEX	O2-MN2	13.82	2.16	2.02
37	V	201	HEM	C3C-C2C	-13.78	1.34	1.45
24	A	409	PHO	CHD-C4C	13.52	1.44	1.35
37	v	201	HEM	C3C-C2C	-13.25	1.35	1.45
37	F	101	HEM	C3C-C2C	-12.94	1.35	1.45
24	A	408	PHO	C1B-CHB	12.83	1.49	1.35
27	B	622	LMG	C25-C24	-12.37	1.50	1.55
20	a	404	OEX	O3-MN3	-12.27	1.86	2.06
37	f	101	HEM	C3C-C2C	-12.10	1.35	1.45
24	A	409	PHO	C4B-CHC	11.99	1.48	1.35
37	F	101	HEM	C3B-C2B	-11.88	1.34	1.45
24	A	409	PHO	C1B-CHB	11.16	1.47	1.35
20	A	401	OEX	O3-MN2	11.14	2.13	2.02
20	A	401	OEX	O3-MN3	11.02	2.24	2.06
24	a	412	PHO	C4B-CHC	11.01	1.47	1.35
24	a	412	PHO	C1B-CHB	10.56	1.47	1.35
27	A	413	LMG	C43-C42	-10.49	1.51	1.55
24	a	413	PHO	C4B-CHC	10.19	1.46	1.35
37	V	201	HEM	C3B-C2B	-10.00	1.35	1.45
37	f	101	HEM	C3B-C2B	-9.86	1.36	1.45
37	v	201	HEM	C3B-C2B	-9.82	1.36	1.45
34	C	516	DGD	CGB-CFB	-9.78	1.51	1.55
23	C	513	CLA	MG-NA	9.76	2.36	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	920	LMG	C43-C42	-9.75	1.51	1.55
23	B	615	CLA	C3B-C4B	9.62	1.52	1.41
27	a	418	LMG	C25-C24	-9.55	1.51	1.55
23	b	612	CLA	C3B-C4B	9.50	1.52	1.41
27	A	413	LMG	C25-C24	-9.22	1.51	1.55
23	c	914	CLA	MG-NC	9.09	2.34	2.07
20	a	404	OEX	O3-MN1	-9.00	1.93	2.02
23	A	406	CLA	C3B-C4B	8.77	1.51	1.41
27	a	418	LMG	C43-C42	-8.75	1.51	1.55
20	a	404	OEX	O2-MN3	-8.73	1.91	2.06
23	C	512	CLA	MG-NA	8.71	2.33	2.07
23	A	407	CLA	C3B-C4B	8.66	1.51	1.41
23	b	608	CLA	C3B-C4B	8.58	1.51	1.41
23	C	501	CLA	C3B-C4B	8.55	1.51	1.41
23	b	611	CLA	C3B-C4B	8.53	1.51	1.41
23	C	511	CLA	MG-NA	8.52	2.32	2.07
24	A	408	PHO	C4B-CHC	8.51	1.44	1.35
27	b	623	LMG	C43-C42	-8.49	1.51	1.55
23	B	616	CLA	MG-NA	8.42	2.32	2.07
23	b	604	CLA	C3B-C4B	8.38	1.51	1.41
23	c	910	CLA	OBD-CAD	8.38	1.34	1.22
27	c	920	LMG	C25-C24	-8.35	1.51	1.55
23	C	504	CLA	C3B-C4B	8.35	1.51	1.41
23	c	912	CLA	C3B-C4B	8.24	1.51	1.41
23	b	610	CLA	C3B-C4B	8.23	1.51	1.41
23	b	616	CLA	C3B-C4B	8.18	1.51	1.41
23	B	607	CLA	MG-NA	8.12	2.31	2.07
37	V	201	HEM	CMB-C2B	8.11	1.58	1.45
27	C	519	LMG	C25-C24	-8.09	1.51	1.55
27	C	519	LMG	C43-C42	-8.07	1.51	1.55
23	B	602	CLA	C3B-C4B	8.07	1.51	1.41
23	D	402	CLA	C3B-C4B	8.03	1.50	1.41
23	b	615	CLA	MG-NA	8.03	2.31	2.07
23	b	605	CLA	C3B-C4B	7.97	1.50	1.41
23	b	609	CLA	MG-NA	7.94	2.30	2.07
23	B	611	CLA	C3B-C4B	7.92	1.50	1.41
26	A	412	SQD	C6-S	-7.90	1.66	1.77
23	C	503	CLA	C3B-C4B	7.85	1.50	1.41
23	c	909	CLA	C3B-C4B	7.72	1.50	1.41
23	C	507	CLA	MG-NA	7.61	2.29	2.07
23	b	607	CLA	C3B-C4B	7.60	1.50	1.41
23	b	609	CLA	C3B-C4B	7.58	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C3B-C2B	7.55	1.49	1.40
23	c	904	CLA	MG-NA	7.54	2.29	2.07
23	c	906	CLA	C3B-C4B	7.50	1.50	1.41
26	a	416	SQD	C6-S	-7.48	1.67	1.77
23	B	606	CLA	C3B-C4B	7.43	1.50	1.41
23	C	506	CLA	MG-NA	7.42	2.29	2.07
23	C	513	CLA	C3B-C4B	7.37	1.50	1.41
34	C	517	DGD	CGA-CFA	-7.32	1.52	1.55
20	A	401	OEX	O2-MN3	-7.32	1.93	2.06
23	c	905	CLA	C3B-C4B	7.31	1.50	1.41
26	a	401	SQD	C6-S	-7.28	1.67	1.77
23	b	615	CLA	C3B-C4B	7.27	1.50	1.41
23	b	614	CLA	C3B-C4B	7.23	1.49	1.41
23	A	407	CLA	MG-NA	7.22	2.28	2.07
23	C	502	CLA	C3B-C4B	7.21	1.49	1.41
23	c	913	CLA	C3B-C4B	7.20	1.49	1.41
23	B	610	CLA	C3B-C4B	7.20	1.49	1.41
23	b	606	CLA	C3B-C4B	7.14	1.49	1.41
23	c	913	CLA	MG-NA	7.13	2.28	2.07
23	c	914	CLA	C3B-C4B	7.08	1.49	1.41
23	B	602	CLA	MG-NA	7.06	2.28	2.07
23	B	608	CLA	C3B-C4B	7.05	1.49	1.41
23	B	603	CLA	C3B-C4B	7.04	1.49	1.41
23	c	907	CLA	MG-ND	-7.00	1.89	2.05
23	B	613	CLA	C3B-C4B	6.97	1.49	1.41
23	C	508	CLA	MG-NA	6.96	2.27	2.07
27	Z	101	LMG	C43-C42	-6.95	1.52	1.55
23	C	512	CLA	C3B-C4B	6.95	1.49	1.41
36	D	410	LHG	C35-C34	-6.94	1.52	1.55
37	V	201	HEM	CMC-C2C	6.93	1.56	1.45
23	b	618	CLA	C3B-C4B	6.93	1.49	1.41
23	B	613	CLA	MG-NA	6.91	2.27	2.07
23	c	914	CLA	MG-ND	6.91	2.20	2.05
23	C	509	CLA	MG-NA	6.90	2.27	2.07
23	c	909	CLA	MG-NA	6.86	2.27	2.07
23	C	513	CLA	C3B-C2B	6.85	1.49	1.40
23	C	505	CLA	C3B-C4B	6.85	1.49	1.41
27	c	921	LMG	C43-C42	-6.79	1.52	1.55
23	a	414	CLA	C3B-C4B	6.78	1.49	1.41
23	c	905	CLA	MG-NA	6.76	2.27	2.07
23	b	619	CLA	C3B-C4B	6.75	1.49	1.41
27	b	623	LMG	C25-C24	-6.72	1.52	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C3B-C4B	6.66	1.49	1.41
37	v	201	HEM	CMC-C2C	6.64	1.56	1.45
23	B	604	CLA	C3B-C4B	6.64	1.49	1.41
23	c	904	CLA	MG-NC	6.62	2.26	2.07
23	D	403	CLA	C3B-C4B	6.62	1.49	1.41
23	B	612	CLA	C3B-C4B	6.59	1.49	1.41
23	C	507	CLA	C3B-C4B	6.58	1.49	1.41
23	B	617	CLA	C3B-C4B	6.58	1.49	1.41
27	d	410	LMG	C25-C24	-6.56	1.52	1.55
23	c	914	CLA	C3B-C2B	6.53	1.48	1.40
23	D	402	CLA	CHB-C4A	6.51	1.42	1.33
23	c	902	CLA	C3B-C2B	6.50	1.48	1.40
23	C	508	CLA	C3B-C2B	6.50	1.48	1.40
23	C	511	CLA	C3B-C4B	6.50	1.49	1.41
23	B	605	CLA	MG-NA	6.49	2.26	2.07
34	H	102	DGD	CGA-CFA	-6.48	1.52	1.55
37	f	101	HEM	CMB-C2B	6.45	1.56	1.45
23	B	603	CLA	C1B-C2B	6.43	1.53	1.43
34	C	516	DGD	CGA-CFA	-6.42	1.52	1.55
27	D	411	LMG	C25-C24	-6.41	1.52	1.55
23	b	618	CLA	MG-NA	6.40	2.26	2.07
27	B	622	LMG	C43-C42	-6.40	1.52	1.55
23	C	510	CLA	MG-NA	6.40	2.26	2.07
23	B	603	CLA	MG-NA	6.39	2.26	2.07
23	b	614	CLA	MG-NA	6.38	2.26	2.07
24	A	409	PHO	C3B-C2B	6.37	1.48	1.40
20	a	404	OEX	O2-MN2	-6.36	1.96	2.02
23	B	605	CLA	C3B-C4B	6.32	1.48	1.41
26	A	418	SQD	C6-S	-6.32	1.68	1.77
23	B	609	CLA	C3B-C4B	6.31	1.48	1.41
23	a	410	CLA	C3B-C4B	6.31	1.48	1.41
23	b	607	CLA	MG-NA	6.30	2.25	2.07
23	d	402	CLA	C3B-C4B	6.28	1.48	1.41
27	d	410	LMG	C43-C42	-6.28	1.52	1.55
23	b	609	CLA	C3B-C2B	6.27	1.48	1.40
23	c	903	CLA	MG-ND	-6.27	1.91	2.05
23	c	910	CLA	C3B-C4B	6.26	1.48	1.41
23	C	503	CLA	MG-NC	6.25	2.25	2.07
23	B	603	CLA	C3B-C2B	6.22	1.48	1.40
23	c	910	CLA	MG-ND	-6.22	1.91	2.05
23	A	410	CLA	C3B-C4B	6.21	1.48	1.41
23	b	613	CLA	C3B-C4B	6.21	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	912	CLA	MG-NA	6.21	2.25	2.07
23	c	902	CLA	MG-NA	6.20	2.25	2.07
37	f	101	HEM	CMC-C2C	6.17	1.55	1.45
23	c	908	CLA	C3B-C4B	6.15	1.48	1.41
23	A	406	CLA	OBD-CAD	6.12	1.31	1.22
23	c	903	CLA	C3B-C4B	6.12	1.48	1.41
23	c	913	CLA	MG-NB	6.12	2.18	2.05
23	b	605	CLA	OBD-CAD	6.11	1.31	1.22
34	c	919	DGD	CGB-CFB	-6.10	1.52	1.55
23	C	506	CLA	C3B-C4B	6.09	1.48	1.41
23	a	411	CLA	C3B-C4B	6.08	1.48	1.41
37	F	101	HEM	CMC-C2C	6.07	1.55	1.45
23	c	903	CLA	C3B-C2B	6.07	1.48	1.40
23	C	508	CLA	C3C-C2C	6.06	1.49	1.36
23	d	403	CLA	C3B-C2B	6.06	1.48	1.40
20	A	401	OEX	O1-MN2	6.02	2.08	2.02
23	b	610	CLA	C3C-C2C	6.00	1.49	1.36
23	c	907	CLA	MG-NB	5.99	2.18	2.05
23	C	503	CLA	C3B-C2B	5.99	1.47	1.40
23	C	508	CLA	MG-NB	5.98	2.18	2.05
34	h	102	DGD	CGB-CFB	-5.97	1.52	1.55
23	c	912	CLA	C3B-C2B	5.97	1.47	1.40
23	C	506	CLA	C3B-C2B	5.95	1.47	1.40
23	c	910	CLA	MG-NA	5.93	2.24	2.07
37	V	201	HEM	CMD-C2D	5.93	1.55	1.45
23	a	409	CLA	OBD-CAD	5.92	1.30	1.22
23	B	607	CLA	C3B-C2B	5.92	1.47	1.40
23	c	907	CLA	C3B-C4B	5.92	1.48	1.41
23	c	905	CLA	C3C-C2C	5.90	1.49	1.36
37	v	201	HEM	CMD-C2D	5.88	1.55	1.45
23	b	605	CLA	C3C-C2C	5.88	1.49	1.36
23	B	603	CLA	C3C-C2C	5.87	1.49	1.36
23	b	615	CLA	C1B-C2B	5.86	1.52	1.43
23	b	611	CLA	MG-NA	5.85	2.24	2.07
23	c	904	CLA	C3B-C4B	5.83	1.48	1.41
23	B	616	CLA	C3B-C4B	5.82	1.48	1.41
34	c	918	DGD	CGA-CFA	-5.82	1.52	1.55
23	c	905	CLA	MG-ND	-5.82	1.92	2.05
23	c	908	CLA	MG-ND	5.80	2.17	2.05
23	D	403	CLA	MG-NA	5.78	2.24	2.07
37	F	101	HEM	CMB-C2B	5.78	1.54	1.45
23	c	913	CLA	C3C-C2C	5.77	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C3B-C4B	5.75	1.48	1.41
23	c	911	CLA	C3B-C4B	5.75	1.48	1.41
23	a	409	CLA	C3B-C4B	5.75	1.48	1.41
24	A	408	PHO	C3B-C2B	5.75	1.47	1.40
23	c	913	CLA	C3B-C2B	5.73	1.47	1.40
23	b	604	CLA	MG-NC	5.72	2.24	2.07
37	v	201	HEM	C3B-CAB	5.68	1.58	1.40
23	c	903	CLA	OBD-CAD	5.68	1.30	1.22
23	C	504	CLA	C3B-C2B	5.65	1.47	1.40
23	c	903	CLA	MG-NA	5.61	2.23	2.07
23	b	618	CLA	OBD-CAD	5.61	1.30	1.22
27	Z	101	LMG	C25-C24	-5.60	1.52	1.55
23	b	613	CLA	C3C-C2C	5.59	1.48	1.36
27	D	411	LMG	C43-C42	-5.57	1.52	1.55
23	c	904	CLA	C3B-C2B	5.56	1.47	1.40
26	B	621	SQD	C6-S	-5.55	1.69	1.77
23	C	513	CLA	C3C-C2C	5.55	1.48	1.36
23	b	604	CLA	C3B-C2B	5.53	1.47	1.40
23	c	907	CLA	C3B-C2B	5.52	1.47	1.40
23	c	910	CLA	C3B-C2B	5.50	1.47	1.40
23	B	614	CLA	C3B-C4B	5.48	1.47	1.41
23	d	403	CLA	C3B-C4B	5.48	1.47	1.41
23	b	615	CLA	C3C-C2C	5.47	1.48	1.36
23	b	605	CLA	C3B-C2B	5.47	1.47	1.40
23	c	908	CLA	C3C-C2C	5.47	1.48	1.36
23	c	904	CLA	C3C-C2C	5.43	1.48	1.36
23	b	610	CLA	MG-NA	5.40	2.23	2.07
23	B	614	CLA	MG-NA	5.40	2.23	2.07
23	B	608	CLA	MG-NA	5.39	2.23	2.07
23	B	612	CLA	C4A-NA	-5.37	1.29	1.38
23	b	612	CLA	C3C-C2C	5.35	1.48	1.36
37	v	201	HEM	CMB-C2B	5.35	1.54	1.45
23	d	403	CLA	C3C-C2C	5.33	1.48	1.36
23	c	912	CLA	OBD-CAD	5.32	1.30	1.22
23	b	612	CLA	O2D-CGD	5.32	1.47	1.33
23	c	909	CLA	C3B-C2B	5.32	1.47	1.40
23	C	512	CLA	C3C-C2C	5.31	1.48	1.36
34	C	518	DGD	CGB-CFB	-5.29	1.53	1.55
24	a	412	PHO	C3C-C2C	5.29	1.48	1.36
23	c	909	CLA	O2D-CGD	5.28	1.46	1.33
24	A	408	PHO	CHA-C1A	5.28	1.49	1.37
37	V	201	HEM	C3B-CAB	5.27	1.57	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	MG-NB	-5.27	1.93	2.05
23	C	507	CLA	C3C-C2C	5.26	1.48	1.36
23	c	906	CLA	C3B-C2B	5.26	1.47	1.40
23	B	602	CLA	O2A-CGA	5.25	1.49	1.33
37	f	101	HEM	CMD-C2D	5.24	1.54	1.45
23	B	602	CLA	C3B-C2B	5.24	1.46	1.40
23	C	503	CLA	C3C-C2C	5.23	1.48	1.36
23	b	606	CLA	C3C-C2C	5.23	1.48	1.36
23	B	606	CLA	C3C-C2C	5.22	1.48	1.36
23	c	914	CLA	C3C-C2C	5.21	1.47	1.36
23	B	604	CLA	MG-NA	5.19	2.22	2.07
23	C	504	CLA	MG-NC	5.17	2.22	2.07
26	L	103	SQD	C6-S	-5.17	1.70	1.77
34	c	917	DGD	CGA-CFA	-5.16	1.53	1.55
23	c	907	CLA	O2D-CGD	5.15	1.46	1.33
23	C	510	CLA	C3C-C2C	5.14	1.47	1.36
23	D	402	CLA	C3B-C2B	5.13	1.46	1.40
23	c	913	CLA	O2D-CGD	5.13	1.46	1.33
23	c	909	CLA	C3C-C2C	5.12	1.47	1.36
23	a	414	CLA	C3B-C2B	5.12	1.46	1.40
23	B	617	CLA	C3C-C2C	5.12	1.47	1.36
23	B	612	CLA	MG-NA	5.12	2.22	2.07
37	F	101	HEM	CMD-C2D	5.12	1.53	1.45
23	b	612	CLA	MG-NC	5.12	2.22	2.07
23	b	611	CLA	C3B-C2B	5.11	1.46	1.40
23	c	902	CLA	C3B-C4B	5.10	1.47	1.41
30	z	101	LMT	C5-C6	-5.10	1.53	1.55
23	b	611	CLA	OBD-CAD	5.09	1.29	1.22
23	b	619	CLA	C3B-C2B	5.08	1.46	1.40
23	C	510	CLA	C3B-C4B	5.08	1.47	1.41
23	B	612	CLA	CHB-C4A	5.08	1.40	1.33
24	A	409	PHO	CHA-C1A	5.06	1.49	1.37
23	C	509	CLA	OBD-CAD	5.06	1.29	1.22
23	C	505	CLA	C3C-C2C	5.05	1.47	1.36
23	b	607	CLA	C3C-C2C	5.03	1.47	1.36
23	A	406	CLA	CHB-C4A	5.02	1.40	1.33
23	b	618	CLA	C3B-C2B	5.00	1.46	1.40
23	C	501	CLA	C3B-C2B	5.00	1.46	1.40
23	B	607	CLA	C3C-C2C	5.00	1.47	1.36
23	B	606	CLA	MG-NA	4.99	2.22	2.07
23	b	604	CLA	O2D-CGD	4.98	1.46	1.33
23	b	610	CLA	C1B-C2B	4.98	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	617	CLA	C3B-C2B	4.97	1.46	1.40
23	c	908	CLA	MG-NA	4.96	2.21	2.07
23	b	618	CLA	C3C-C2C	4.95	1.47	1.36
23	C	512	CLA	C3B-C2B	4.93	1.46	1.40
37	v	201	HEM	C3C-CAC	4.92	1.56	1.40
23	c	908	CLA	MG-NC	4.89	2.21	2.07
23	c	911	CLA	MG-NC	4.89	2.21	2.07
34	d	406	DGD	O1G-C1A	4.89	1.48	1.33
37	F	101	HEM	C3B-CAB	4.88	1.56	1.40
23	B	616	CLA	C3C-C2C	4.88	1.47	1.36
23	b	604	CLA	O2A-CGA	4.87	1.48	1.33
37	F	101	HEM	FE-NC	4.86	2.15	1.95
23	c	914	CLA	O2D-CGD	4.85	1.45	1.33
23	b	613	CLA	O2D-CGD	4.85	1.45	1.33
23	B	614	CLA	C3C-C2C	4.84	1.47	1.36
23	b	613	CLA	OBD-CAD	4.84	1.29	1.22
36	a	417	LHG	C29-C28	-4.84	1.53	1.55
23	c	906	CLA	MG-NA	4.83	2.21	2.07
23	B	608	CLA	C3B-C2B	4.83	1.46	1.40
23	b	612	CLA	CHC-C1C	4.82	1.51	1.35
34	D	406	DGD	O2G-C1B	4.82	1.48	1.34
23	c	907	CLA	C3C-C2C	4.82	1.47	1.36
26	A	418	SQD	O48-C23	4.81	1.48	1.33
23	A	410	CLA	C3C-C2C	4.81	1.47	1.36
23	b	608	CLA	C3C-C2C	4.80	1.47	1.36
24	a	412	PHO	CHA-C1A	4.79	1.48	1.37
23	a	409	CLA	C3B-C2B	4.79	1.46	1.40
23	c	911	CLA	O2D-CGD	4.79	1.45	1.33
23	a	410	CLA	C3C-C2C	4.79	1.47	1.36
23	B	610	CLA	C3C-C2C	4.79	1.47	1.36
27	Z	101	LMG	O7-C10	4.78	1.48	1.34
23	C	508	CLA	O2D-CGD	4.78	1.45	1.33
26	D	407	SQD	O47-C7	4.78	1.48	1.34
23	c	911	CLA	C3B-C2B	4.78	1.46	1.40
23	B	609	CLA	MG-NB	-4.78	1.94	2.05
23	C	505	CLA	C1B-C2B	4.78	1.51	1.43
23	c	912	CLA	O2D-CGD	4.77	1.45	1.33
23	b	619	CLA	C3C-C2C	4.76	1.47	1.36
23	C	502	CLA	O2D-CGD	4.76	1.45	1.33
23	a	410	CLA	MG-NA	4.76	2.21	2.07
23	a	409	CLA	MG-NA	4.75	2.21	2.07
23	d	402	CLA	C3B-C2B	4.75	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	O2D-CGD	4.75	1.45	1.33
23	b	616	CLA	O2D-CGD	4.75	1.45	1.33
23	c	903	CLA	O2D-CGD	4.75	1.45	1.33
23	A	405	CLA	C3B-C4B	4.75	1.46	1.41
23	B	602	CLA	C3C-C2C	4.74	1.46	1.36
23	c	914	CLA	OBD-CAD	4.74	1.29	1.22
23	C	511	CLA	O2D-CGD	4.73	1.45	1.33
23	c	911	CLA	C3C-C2C	4.73	1.46	1.36
37	f	101	HEM	C3B-CAB	4.72	1.55	1.40
23	b	608	CLA	O2D-CGD	4.71	1.45	1.33
37	V	201	HEM	C3C-CAC	4.71	1.55	1.40
23	D	402	CLA	C4A-NA	-4.71	1.30	1.38
23	A	407	CLA	OBD-CAD	4.70	1.29	1.22
23	B	615	CLA	MG-NA	4.70	2.21	2.07
23	b	609	CLA	C3C-C2C	4.69	1.46	1.36
26	a	401	SQD	O47-C7	4.70	1.48	1.34
23	C	508	CLA	MG-NC	4.69	2.21	2.07
23	b	612	CLA	C1B-C2B	4.69	1.51	1.43
23	D	403	CLA	C3C-C2C	4.68	1.46	1.36
23	D	402	CLA	C1B-C2B	4.68	1.51	1.43
23	a	409	CLA	C3C-C2C	4.67	1.46	1.36
23	C	510	CLA	C3B-C2B	4.65	1.46	1.40
23	b	605	CLA	C1B-C2B	4.65	1.50	1.43
23	C	510	CLA	OBD-CAD	4.64	1.29	1.22
27	c	921	LMG	O7-C10	4.64	1.48	1.34
23	b	605	CLA	MG-NC	4.63	2.20	2.07
23	b	618	CLA	CHB-C4A	4.63	1.39	1.33
23	c	910	CLA	O2D-CGD	4.62	1.45	1.33
23	B	607	CLA	O2D-CGD	4.62	1.45	1.33
20	a	404	OEX	O1-MN2	4.62	2.07	2.02
23	C	509	CLA	C3B-C4B	4.61	1.46	1.41
24	a	413	PHO	C3B-C2B	4.61	1.46	1.40
23	A	405	CLA	C3C-C2C	4.60	1.46	1.36
23	d	403	CLA	MG-NA	4.59	2.20	2.07
23	a	414	CLA	C3C-C2C	4.59	1.46	1.36
23	C	505	CLA	O2D-CGD	4.59	1.45	1.33
23	B	610	CLA	MG-NB	4.59	2.15	2.05
23	C	509	CLA	O2D-CGD	4.58	1.45	1.33
23	b	604	CLA	C3C-C2C	4.57	1.46	1.36
23	B	603	CLA	CHC-C1C	4.56	1.50	1.35
23	b	613	CLA	MG-NA	4.56	2.20	2.07
23	B	613	CLA	CHC-C1C	4.55	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	PHO	OBD-CAD	4.54	1.28	1.22
23	b	610	CLA	CHC-C1C	4.54	1.50	1.35
26	f	102	SQD	O48-C23	4.54	1.47	1.33
26	L	103	SQD	O47-C7	4.53	1.48	1.34
26	B	621	SQD	O47-C7	4.53	1.48	1.34
36	a	417	LHG	O8-C23	4.52	1.47	1.33
23	B	606	CLA	O2D-CGD	4.52	1.44	1.33
23	b	619	CLA	CHC-C1C	4.52	1.50	1.35
23	b	617	CLA	C3B-C4B	4.51	1.46	1.41
23	C	511	CLA	C3B-C2B	4.51	1.46	1.40
23	b	614	CLA	C3B-C2B	4.51	1.46	1.40
23	A	410	CLA	OBD-CAD	4.50	1.28	1.22
23	c	912	CLA	C3C-C2C	4.49	1.46	1.36
24	a	412	PHO	O2D-CGD	4.50	1.44	1.33
23	b	619	CLA	O2D-CGD	4.49	1.44	1.33
23	C	502	CLA	CHC-C1C	4.49	1.50	1.35
23	b	606	CLA	OBD-CAD	4.49	1.28	1.22
23	C	509	CLA	C3C-C2C	4.48	1.46	1.36
23	b	616	CLA	MG-NA	4.47	2.20	2.07
23	b	616	CLA	OBD-CAD	4.47	1.28	1.22
23	C	505	CLA	C3B-C2B	4.46	1.46	1.40
27	B	622	LMG	O8-C28	4.46	1.46	1.33
23	C	512	CLA	O2D-CGD	4.45	1.44	1.33
23	B	608	CLA	C3C-C2C	4.44	1.46	1.36
28	d	405	PL9	C7-C3	4.44	1.55	1.51
34	D	406	DGD	O1G-C1A	4.43	1.46	1.33
23	A	407	CLA	C3C-C2C	4.43	1.46	1.36
26	a	401	SQD	O48-C23	4.43	1.46	1.33
23	B	615	CLA	C1C-NC	-4.43	1.29	1.37
23	c	905	CLA	C3B-C2B	4.43	1.45	1.40
24	a	412	PHO	C3B-C2B	4.43	1.45	1.40
23	d	402	CLA	MG-NB	-4.43	1.95	2.05
23	c	909	CLA	MG-NC	4.42	2.20	2.07
23	B	611	CLA	MG-NA	4.42	2.20	2.07
27	c	921	LMG	C25-C24	-4.41	1.53	1.55
27	c	920	LMG	O8-C28	4.41	1.46	1.33
23	C	513	CLA	O2D-CGD	4.41	1.44	1.33
23	B	616	CLA	C1B-C2B	4.40	1.50	1.43
23	d	402	CLA	O2A-CGA	4.40	1.46	1.33
23	d	402	CLA	C3C-C2C	4.40	1.46	1.36
24	a	413	PHO	C3C-C2C	4.40	1.46	1.36
23	B	615	CLA	MG-NC	4.40	2.20	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	f	101	HEM	C3C-CAC	4.40	1.54	1.40
23	C	506	CLA	O2D-CGD	4.39	1.44	1.33
23	D	403	CLA	C3B-C2B	4.39	1.45	1.40
23	b	616	CLA	C3C-C2C	4.38	1.46	1.36
23	C	501	CLA	MG-NB	4.38	2.14	2.05
23	b	612	CLA	C3B-C2B	4.38	1.45	1.40
23	B	609	CLA	C3C-C2C	4.37	1.46	1.36
23	D	403	CLA	MG-NC	4.37	2.20	2.07
23	B	605	CLA	C1B-C2B	4.36	1.50	1.43
37	v	201	HEM	FE-ND	4.36	2.13	1.95
23	C	504	CLA	C3C-C2C	4.36	1.46	1.36
36	E	101	LHG	O8-C23	4.36	1.46	1.33
23	A	410	CLA	MG-NB	-4.35	1.95	2.05
26	D	407	SQD	C6-S	-4.35	1.71	1.77
23	b	618	CLA	O2D-CGD	4.35	1.44	1.33
23	C	502	CLA	C3B-C2B	4.35	1.45	1.40
23	b	616	CLA	C3B-C2B	4.35	1.45	1.40
36	a	417	LHG	O7-C7	4.35	1.47	1.34
23	B	610	CLA	C1B-C2B	4.35	1.50	1.43
23	B	615	CLA	CHC-C1C	4.34	1.49	1.35
23	c	902	CLA	C3C-C2C	4.33	1.46	1.36
23	b	619	CLA	MG-NA	4.32	2.20	2.07
23	b	606	CLA	O2D-CGD	4.32	1.44	1.33
23	B	605	CLA	C3C-C2C	4.31	1.46	1.36
23	b	612	CLA	MG-NB	4.30	2.14	2.05
27	c	921	LMG	O8-C28	4.30	1.46	1.33
23	D	403	CLA	MG-NB	-4.30	1.95	2.05
23	B	613	CLA	C3C-C2C	4.30	1.45	1.36
23	a	411	CLA	C3C-C2C	4.29	1.45	1.36
23	c	905	CLA	O2D-CGD	4.29	1.44	1.33
23	C	502	CLA	C3C-C2C	4.29	1.45	1.36
23	A	406	CLA	C3C-C2C	4.28	1.45	1.36
23	C	511	CLA	C3C-C2C	4.28	1.45	1.36
23	c	914	CLA	O2A-CGA	4.27	1.46	1.33
23	c	911	CLA	OBD-CAD	4.26	1.28	1.22
34	H	102	DGD	O5D-C1E	4.26	1.47	1.40
23	c	906	CLA	C1B-C2B	4.26	1.50	1.43
23	b	606	CLA	MG-NA	4.26	2.19	2.07
26	D	407	SQD	O48-C23	4.26	1.46	1.33
23	c	914	CLA	CHC-C1C	4.25	1.49	1.35
23	b	611	CLA	C3C-C2C	4.25	1.45	1.36
23	B	610	CLA	C3B-C2B	4.25	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	O2D-CGD	4.24	1.44	1.33
23	b	614	CLA	O2D-CGD	4.24	1.44	1.33
23	b	610	CLA	MG-NC	4.24	2.19	2.07
23	B	607	CLA	CHC-C1C	4.24	1.49	1.35
27	C	519	LMG	O8-C28	4.23	1.46	1.33
23	B	603	CLA	MG-NB	4.23	2.14	2.05
23	c	910	CLA	C3C-C2C	4.23	1.45	1.36
24	a	413	PHO	CHA-C1A	4.22	1.47	1.37
23	A	405	CLA	CHC-C1C	4.22	1.49	1.35
23	B	611	CLA	C3C-C2C	4.21	1.45	1.36
27	Z	101	LMG	O8-C28	4.21	1.46	1.33
37	f	101	HEM	FE-NB	4.21	2.10	1.95
23	b	617	CLA	O2A-CGA	4.20	1.46	1.33
23	a	414	CLA	OBD-CAD	4.20	1.28	1.22
27	A	413	LMG	O7-C10	4.20	1.47	1.34
23	b	612	CLA	OBD-CAD	4.20	1.28	1.22
23	C	506	CLA	O2A-CGA	4.19	1.46	1.33
23	C	501	CLA	OBD-CAD	4.18	1.28	1.22
23	c	913	CLA	O2A-CGA	4.18	1.46	1.33
23	B	616	CLA	OBD-CAD	4.18	1.28	1.22
27	c	920	LMG	O7-C10	4.17	1.46	1.34
23	b	604	CLA	MG-NA	4.16	2.19	2.07
23	b	606	CLA	CHC-C1C	4.15	1.49	1.35
23	b	609	CLA	O2D-CGD	4.15	1.43	1.33
23	a	410	CLA	CHC-C1C	4.15	1.49	1.35
23	C	510	CLA	O2D-CGD	4.15	1.43	1.33
23	B	604	CLA	C3C-C2C	4.13	1.45	1.36
23	c	908	CLA	OBD-CAD	4.12	1.28	1.22
23	b	607	CLA	CHC-C1C	4.12	1.49	1.35
23	C	503	CLA	O2A-CGA	4.12	1.45	1.33
23	C	501	CLA	C3C-C2C	4.11	1.45	1.36
23	C	506	CLA	C3C-C2C	4.10	1.45	1.36
23	c	906	CLA	C3C-C2C	4.10	1.45	1.36
23	B	606	CLA	CHC-C1C	4.10	1.48	1.35
23	B	616	CLA	O2D-CGD	4.10	1.43	1.33
34	d	406	DGD	O2G-C1B	4.10	1.46	1.34
23	b	619	CLA	O2A-CGA	4.09	1.45	1.33
23	C	513	CLA	MG-NB	4.09	2.14	2.05
23	D	402	CLA	O2A-CGA	4.09	1.45	1.33
23	d	402	CLA	CHC-C1C	4.08	1.48	1.35
23	C	501	CLA	CHC-C1C	4.08	1.48	1.35
37	F	101	HEM	C3C-CAC	4.07	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3B-C2B	4.07	1.45	1.40
23	c	904	CLA	O2D-CGD	4.06	1.43	1.33
27	a	418	LMG	O7-C10	4.06	1.46	1.34
23	C	508	CLA	CHC-C1C	4.06	1.48	1.35
23	D	402	CLA	OBD-CAD	4.06	1.28	1.22
23	b	618	CLA	C1B-C2B	4.06	1.50	1.43
23	c	905	CLA	MG-NC	4.05	2.19	2.07
27	A	413	LMG	O8-C28	4.05	1.45	1.33
23	A	405	CLA	O2D-CGD	4.05	1.43	1.33
23	b	616	CLA	O2A-CGA	4.04	1.45	1.33
23	A	406	CLA	C1B-C2B	4.04	1.50	1.43
23	b	617	CLA	MG-NA	4.04	2.19	2.07
23	B	611	CLA	CHC-C1C	4.04	1.48	1.35
24	a	413	PHO	O2D-CGD	4.03	1.43	1.33
23	c	913	CLA	CHC-C1C	4.03	1.48	1.35
36	E	101	LHG	O7-C7	4.03	1.46	1.34
34	d	406	DGD	CGB-CFB	-4.02	1.53	1.55
23	D	403	CLA	C1B-CHB	4.02	1.50	1.39
23	C	512	CLA	CHC-C1C	4.02	1.48	1.35
23	B	617	CLA	OBD-CAD	4.02	1.28	1.22
23	B	604	CLA	C3B-C2B	4.02	1.45	1.40
23	B	606	CLA	C3B-C2B	4.01	1.45	1.40
23	b	605	CLA	CHC-C1C	4.00	1.48	1.35
23	b	616	CLA	CHB-C4A	3.99	1.38	1.33
23	C	511	CLA	C1B-CHB	3.98	1.50	1.39
23	A	410	CLA	C3B-C2B	3.98	1.45	1.40
26	A	418	SQD	O47-C7	3.98	1.46	1.34
23	b	614	CLA	C3C-C2C	3.98	1.45	1.36
34	C	518	DGD	CGA-CFA	-3.97	1.53	1.55
23	A	410	CLA	CHC-C1C	3.97	1.48	1.35
23	C	505	CLA	MG-NB	3.97	2.13	2.05
23	B	610	CLA	CHC-C1C	3.97	1.48	1.35
23	C	503	CLA	CHC-C1C	3.97	1.48	1.35
23	d	403	CLA	O2A-CGA	3.96	1.45	1.33
23	c	904	CLA	CHC-C1C	3.96	1.48	1.35
23	b	609	CLA	MG-NC	3.96	2.18	2.07
23	A	405	CLA	OBD-CAD	3.95	1.28	1.22
23	B	616	CLA	C3B-C2B	3.95	1.45	1.40
23	B	614	CLA	CHC-C1C	3.95	1.48	1.35
23	A	405	CLA	MG-NA	3.94	2.18	2.07
23	b	608	CLA	CHC-C1C	3.94	1.48	1.35
20	A	401	OEX	O5-MN3	3.94	2.28	2.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	918	DGD	O1G-C1A	3.93	1.45	1.33
23	C	509	CLA	O2A-CGA	3.93	1.45	1.33
23	D	402	CLA	C4C-C3C	3.92	1.52	1.45
23	D	403	CLA	CHC-C1C	3.92	1.48	1.35
23	B	617	CLA	CHC-C1C	3.91	1.48	1.35
23	B	602	CLA	OBD-CAD	3.91	1.27	1.22
23	b	604	CLA	MG-ND	3.90	2.13	2.05
23	B	609	CLA	C3B-C2B	3.90	1.45	1.40
23	b	619	CLA	MG-ND	3.90	2.13	2.05
23	B	604	CLA	OBD-CAD	3.90	1.27	1.22
23	B	607	CLA	OBD-CAD	3.89	1.27	1.22
23	b	619	CLA	OBD-CAD	3.89	1.27	1.22
23	c	908	CLA	CHC-C1C	3.88	1.48	1.35
23	B	615	CLA	C3C-C2C	3.88	1.45	1.36
23	a	414	CLA	CHC-C1C	3.87	1.48	1.35
23	b	610	CLA	MG-NB	3.87	2.13	2.05
23	c	905	CLA	OBD-CAD	3.87	1.27	1.22
24	A	409	PHO	C3C-C2C	3.87	1.45	1.36
23	C	504	CLA	CHD-C4C	3.87	1.50	1.41
23	B	614	CLA	MG-ND	3.87	2.13	2.05
23	b	616	CLA	CHC-C1C	3.87	1.48	1.35
23	c	913	CLA	MG-NC	3.87	2.18	2.07
23	b	610	CLA	CHB-C4A	3.86	1.38	1.33
23	D	403	CLA	O2A-CGA	3.86	1.45	1.33
34	d	406	DGD	CGA-CFA	-3.86	1.53	1.55
23	b	610	CLA	C3D-C2D	3.86	1.49	1.40
23	b	610	CLA	O2D-CGD	3.85	1.43	1.33
27	a	418	LMG	O8-C28	3.85	1.45	1.33
23	B	608	CLA	CHB-C4A	3.85	1.38	1.33
23	D	402	CLA	O2D-CGD	3.85	1.43	1.33
23	C	505	CLA	MG-NA	3.85	2.18	2.07
23	b	604	CLA	CHC-C1C	3.84	1.48	1.35
23	c	902	CLA	OBD-CAD	3.84	1.27	1.22
27	b	623	LMG	O8-C28	3.84	1.45	1.33
30	B	623	LMT	O6B-C6B	3.83	1.59	1.42
23	c	907	CLA	O2A-CGA	3.82	1.45	1.33
23	b	617	CLA	C3B-C2B	3.82	1.45	1.40
23	b	607	CLA	O2D-CGD	3.82	1.43	1.33
23	b	604	CLA	OBD-CAD	3.82	1.27	1.22
37	f	101	HEM	FE-NC	3.81	2.10	1.95
23	C	507	CLA	MG-ND	3.81	2.13	2.05
23	C	511	CLA	O2A-CGA	3.81	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	MG-NB	3.80	2.13	2.05
23	c	908	CLA	C3B-C2B	3.80	1.45	1.40
23	c	911	CLA	O2A-CGA	3.79	1.44	1.33
23	C	506	CLA	C1B-CHB	3.79	1.50	1.39
23	C	507	CLA	CHC-C1C	3.78	1.47	1.35
23	B	604	CLA	C1B-C2B	3.78	1.49	1.43
34	h	102	DGD	O5D-C1E	3.78	1.47	1.40
24	A	408	PHO	C3C-C2C	3.77	1.44	1.36
23	c	913	CLA	OBD-CAD	3.77	1.27	1.22
23	b	617	CLA	O2D-CGD	3.76	1.42	1.33
26	D	407	SQD	C13-C12	-3.76	1.53	1.55
23	C	513	CLA	CHC-C1C	3.76	1.47	1.35
23	B	612	CLA	C3C-C2C	3.76	1.44	1.36
23	A	407	CLA	CHC-C1C	3.76	1.47	1.35
23	C	504	CLA	MG-NA	3.76	2.18	2.07
23	b	613	CLA	MG-ND	-3.76	1.96	2.05
23	b	614	CLA	C1B-CHB	3.76	1.50	1.39
23	c	906	CLA	CHC-C1C	3.76	1.47	1.35
23	b	615	CLA	O2D-CGD	3.76	1.42	1.33
23	C	507	CLA	O2D-CGD	3.75	1.42	1.33
23	a	410	CLA	OBD-CAD	3.75	1.27	1.22
23	C	504	CLA	CHB-C4A	3.75	1.38	1.33
23	B	608	CLA	CHC-C1C	3.74	1.47	1.35
23	c	912	CLA	O2A-CGA	3.74	1.44	1.33
23	C	502	CLA	MG-NA	3.74	2.18	2.07
23	A	406	CLA	C3B-C2B	3.73	1.45	1.40
23	b	608	CLA	MG-NA	3.73	2.18	2.07
23	b	607	CLA	C3B-C2B	3.73	1.45	1.40
23	C	508	CLA	C1B-CHB	3.72	1.50	1.39
23	a	414	CLA	MG-NA	3.72	2.18	2.07
23	A	407	CLA	C4A-NA	-3.72	1.32	1.38
33	U	201	HTG	C1'-S1	-3.72	1.77	1.82
23	c	912	CLA	C1B-CHB	3.72	1.50	1.39
23	b	604	CLA	C4B-CHC	3.71	1.50	1.39
23	d	402	CLA	MG-NA	3.71	2.18	2.07
23	c	907	CLA	MG-NA	3.70	2.18	2.07
23	D	403	CLA	OBD-CAD	3.70	1.27	1.22
23	b	604	CLA	C3D-C2D	3.70	1.49	1.40
23	b	618	CLA	C3D-C2D	3.70	1.49	1.40
23	C	509	CLA	CHC-C1C	3.70	1.47	1.35
23	c	912	CLA	MG-ND	3.70	2.13	2.05
23	C	512	CLA	C1B-C2B	3.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C3B-C2B	3.69	1.45	1.40
23	b	606	CLA	C3B-C2B	3.69	1.45	1.40
24	a	413	PHO	C1A-NA	-3.68	1.28	1.37
23	c	902	CLA	O2A-CGA	3.68	1.44	1.33
23	d	403	CLA	MG-NC	3.68	2.18	2.07
23	a	409	CLA	O2D-CGD	3.67	1.42	1.33
23	C	513	CLA	MG-NC	3.67	2.18	2.07
23	b	613	CLA	C4C-C3C	3.67	1.51	1.45
26	A	412	SQD	O47-C7	3.67	1.45	1.34
23	C	502	CLA	OBD-CAD	3.66	1.27	1.22
23	C	512	CLA	O2A-CGA	3.66	1.44	1.33
26	L	103	SQD	O48-C23	3.66	1.44	1.33
23	c	909	CLA	CHC-C1C	3.66	1.47	1.35
23	A	410	CLA	C1B-CHB	3.66	1.49	1.39
23	b	610	CLA	MG-ND	3.66	2.13	2.05
37	V	201	HEM	FE-ND	3.66	2.10	1.95
23	C	506	CLA	CHC-C1C	3.65	1.47	1.35
23	C	511	CLA	C3D-C2D	3.65	1.48	1.40
23	B	616	CLA	O2A-CGA	3.65	1.44	1.33
34	C	517	DGD	O1G-C1A	3.65	1.44	1.33
23	a	411	CLA	CHC-C1C	3.65	1.47	1.35
23	a	414	CLA	C1B-CHB	3.65	1.49	1.39
23	B	613	CLA	OBD-CAD	3.65	1.27	1.22
23	B	610	CLA	MG-NA	3.64	2.18	2.07
23	B	603	CLA	C1B-CHB	3.64	1.49	1.39
23	c	902	CLA	O2D-CGD	3.64	1.42	1.33
23	A	406	CLA	CHC-C1C	3.63	1.47	1.35
23	A	405	CLA	C3B-C2B	3.63	1.44	1.40
23	a	410	CLA	C3B-C2B	3.63	1.44	1.40
24	a	413	PHO	C3D-C4D	-3.63	1.34	1.40
26	B	621	SQD	O48-C23	3.63	1.44	1.33
24	A	409	PHO	O2D-CGD	3.62	1.42	1.33
23	b	605	CLA	CHD-C4C	3.62	1.49	1.41
23	A	410	CLA	C4B-CHC	3.61	1.49	1.39
23	B	616	CLA	CHC-C1C	3.61	1.47	1.35
23	C	503	CLA	O2D-CGD	3.60	1.42	1.33
37	v	201	HEM	C3D-C2D	3.60	1.52	1.43
23	d	403	CLA	MG-NB	-3.60	1.97	2.05
34	c	918	DGD	CGB-CFB	-3.60	1.53	1.55
23	C	505	CLA	OBD-CAD	3.60	1.27	1.22
27	C	519	LMG	O7-C10	3.60	1.45	1.34
23	c	909	CLA	C4C-C3C	3.59	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	OBD-CAD	3.58	1.27	1.22
24	A	409	PHO	C1D-C2D	3.58	1.50	1.44
27	d	410	LMG	O7-C10	3.58	1.45	1.34
23	c	904	CLA	C1B-CHB	3.58	1.49	1.39
23	c	905	CLA	MG-NB	3.58	2.13	2.05
23	b	617	CLA	C3C-C2C	3.57	1.44	1.36
23	b	614	CLA	CHC-C1C	3.57	1.47	1.35
23	C	503	CLA	C1B-C2B	3.57	1.49	1.43
23	C	512	CLA	C3D-C2D	3.57	1.48	1.40
23	b	607	CLA	MG-ND	-3.56	1.97	2.05
23	D	402	CLA	C3C-C2C	3.56	1.44	1.36
26	a	416	SQD	O47-C7	3.56	1.45	1.34
23	A	405	CLA	C4B-CHC	3.56	1.49	1.39
23	B	615	CLA	O2D-CGD	3.56	1.42	1.33
23	D	402	CLA	MG-NA	3.56	2.17	2.07
33	B	624	HTG	C1'-S1	-3.55	1.76	1.81
23	B	615	CLA	C1B-CHB	3.55	1.49	1.39
23	C	511	CLA	OBD-CAD	3.55	1.27	1.22
27	D	411	LMG	O7-C10	3.55	1.45	1.34
23	c	911	CLA	CHC-C1C	3.55	1.47	1.35
23	B	614	CLA	C3D-C2D	3.55	1.48	1.40
23	C	513	CLA	C1B-CHB	3.55	1.49	1.39
23	c	910	CLA	O2A-CGA	3.55	1.44	1.33
23	B	606	CLA	MG-NC	3.54	2.17	2.07
23	a	414	CLA	O2A-CGA	3.54	1.44	1.33
23	B	602	CLA	CHC-C1C	3.54	1.47	1.35
23	C	510	CLA	O2A-CGA	3.54	1.44	1.33
28	a	419	PL9	C7-C3	3.54	1.54	1.51
23	c	909	CLA	C3D-C2D	3.54	1.48	1.40
23	c	906	CLA	CHD-C4C	3.54	1.49	1.41
23	B	603	CLA	OBD-CAD	3.53	1.27	1.22
23	b	611	CLA	CHC-C1C	3.53	1.47	1.35
23	B	604	CLA	O2D-CGD	3.53	1.42	1.33
23	c	902	CLA	C4A-NA	-3.53	1.32	1.38
23	C	506	CLA	MG-NB	3.52	2.12	2.05
23	d	403	CLA	O2D-CGD	3.52	1.42	1.33
23	c	903	CLA	C3C-C2C	3.52	1.44	1.36
23	C	512	CLA	C1B-CHB	3.52	1.49	1.39
23	b	612	CLA	O2A-CGA	3.51	1.44	1.33
23	c	902	CLA	C1B-CHB	3.51	1.49	1.39
23	c	903	CLA	C4A-NA	-3.51	1.32	1.38
23	C	504	CLA	CHC-C1C	3.51	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	410	LHG	O8-C23	3.51	1.44	1.33
26	a	416	SQD	O48-C23	3.51	1.44	1.33
23	a	409	CLA	C1B-C2B	3.50	1.49	1.43
23	a	410	CLA	C1B-C2B	3.50	1.49	1.43
23	b	615	CLA	CHC-C1C	3.49	1.46	1.35
37	V	201	HEM	CMA-C3A	3.49	1.58	1.51
23	a	411	CLA	C3B-C2B	3.49	1.44	1.40
24	A	408	PHO	O2A-CGA	3.49	1.44	1.33
23	c	914	CLA	C3D-C2D	3.48	1.48	1.40
23	B	606	CLA	C1B-CHB	3.48	1.49	1.39
23	c	908	CLA	O2A-CGA	3.48	1.43	1.33
23	c	903	CLA	C1B-CHB	3.48	1.49	1.39
23	B	611	CLA	C3D-C2D	3.48	1.48	1.40
23	d	403	CLA	C4C-C3C	3.48	1.51	1.45
23	C	508	CLA	C4C-C3C	3.47	1.51	1.45
23	B	613	CLA	MG-NB	3.47	2.12	2.05
23	A	407	CLA	C1B-C2B	3.47	1.49	1.43
30	A	419	LMT	O1'-C1'	3.47	1.46	1.40
23	c	914	CLA	C1B-CHB	3.46	1.49	1.39
23	b	618	CLA	CHD-C4C	3.46	1.49	1.41
23	d	403	CLA	CHC-C1C	3.46	1.46	1.35
23	C	513	CLA	C3D-C2D	3.46	1.48	1.40
23	C	505	CLA	CHC-C1C	3.46	1.46	1.35
23	B	604	CLA	C1B-CHB	3.45	1.49	1.39
23	B	604	CLA	CHC-C1C	3.45	1.46	1.35
23	C	510	CLA	MG-ND	-3.45	1.97	2.05
23	c	902	CLA	CHC-C1C	3.44	1.46	1.35
23	B	617	CLA	O2D-CGD	3.44	1.42	1.33
23	C	501	CLA	MG-NA	3.44	2.17	2.07
23	a	414	CLA	C1B-C2B	3.44	1.49	1.43
23	c	908	CLA	C1B-C2B	3.44	1.49	1.43
37	f	101	HEM	C3D-C2D	3.44	1.52	1.43
23	b	608	CLA	OBD-CAD	3.44	1.27	1.22
27	d	410	LMG	O8-C28	3.43	1.43	1.33
23	B	615	CLA	C1B-C2B	3.43	1.49	1.43
25	b	621	BCR	C5-C6	3.43	1.39	1.34
24	a	413	PHO	O2A-CGA	3.42	1.43	1.33
23	c	906	CLA	O2A-CGA	3.42	1.43	1.33
23	d	402	CLA	C3D-C2D	3.42	1.48	1.40
23	b	614	CLA	O2A-CGA	3.41	1.43	1.33
23	b	614	CLA	CHB-C4A	3.41	1.38	1.33
23	c	908	CLA	C3D-C2D	3.41	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	405	PL9	C21-C19	3.40	1.59	1.51
23	c	912	CLA	C1B-C2B	3.40	1.49	1.43
23	b	609	CLA	CHC-C1C	3.40	1.46	1.35
23	C	504	CLA	O2D-CGD	3.39	1.42	1.33
23	b	613	CLA	CHC-C1C	3.39	1.46	1.35
23	c	905	CLA	C1B-CHB	3.39	1.49	1.39
23	c	905	CLA	C3D-C2D	3.39	1.48	1.40
23	c	908	CLA	O2D-CGD	3.39	1.41	1.33
23	C	506	CLA	C1B-C2B	3.38	1.49	1.43
23	c	905	CLA	CHC-C1C	3.38	1.46	1.35
23	c	912	CLA	CHC-C1C	3.38	1.46	1.35
23	c	910	CLA	C4A-NA	-3.38	1.32	1.38
23	B	608	CLA	C1B-CHB	3.37	1.49	1.39
23	a	411	CLA	O2D-CGD	3.37	1.41	1.33
23	B	605	CLA	O2D-CGD	3.37	1.41	1.33
23	c	909	CLA	MG-NB	3.37	2.12	2.05
34	C	518	DGD	O1G-C1A	3.37	1.43	1.33
23	C	511	CLA	CHC-C1C	3.36	1.46	1.35
23	B	613	CLA	O2D-CGD	3.36	1.41	1.33
23	c	906	CLA	MG-ND	3.36	2.12	2.05
23	c	906	CLA	OBD-CAD	3.36	1.27	1.22
23	B	604	CLA	O2A-CGA	3.35	1.43	1.33
34	c	919	DGD	O1G-C1A	3.35	1.43	1.33
23	B	610	CLA	CHB-C4A	3.35	1.37	1.33
23	B	609	CLA	O2A-CGA	3.35	1.43	1.33
33	D	414	HTG	C1'-S1	-3.35	1.76	1.81
23	a	411	CLA	C3D-C2D	3.34	1.48	1.40
23	B	611	CLA	C4A-NA	-3.34	1.32	1.38
23	c	913	CLA	C4B-CHC	3.34	1.49	1.39
23	C	506	CLA	OBD-CAD	3.34	1.27	1.22
23	b	613	CLA	C4A-NA	-3.34	1.32	1.38
23	c	913	CLA	C1B-C2B	3.34	1.49	1.43
23	C	513	CLA	OBD-CAD	3.33	1.27	1.22
23	B	612	CLA	CHC-C1C	3.33	1.46	1.35
23	B	617	CLA	O2A-CGA	3.33	1.43	1.33
23	C	510	CLA	MG-NB	3.33	2.12	2.05
23	c	913	CLA	C3D-C2D	3.33	1.48	1.40
23	C	506	CLA	CHB-C4A	3.33	1.37	1.33
23	a	414	CLA	O2D-CGD	3.32	1.41	1.33
34	H	102	DGD	O1G-C1A	3.32	1.43	1.33
23	c	910	CLA	C1B-C2B	3.32	1.48	1.43
23	b	617	CLA	C1B-CHB	3.32	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C3B-C2B	3.32	1.44	1.40
23	a	411	CLA	C4A-NA	-3.32	1.32	1.38
23	b	615	CLA	CHB-C4A	3.32	1.37	1.33
23	B	604	CLA	C3D-C2D	3.31	1.48	1.40
23	C	508	CLA	C3D-C2D	3.31	1.48	1.40
24	a	412	PHO	OBD-CAD	3.31	1.27	1.22
20	a	404	OEX	O5-MN3	3.31	2.25	2.11
23	C	507	CLA	O2A-CGA	3.31	1.43	1.33
23	d	403	CLA	C4A-NA	-3.31	1.32	1.38
23	B	602	CLA	C4A-NA	-3.30	1.32	1.38
23	A	406	CLA	C4B-CHC	3.30	1.48	1.39
23	B	602	CLA	C4B-CHC	3.30	1.48	1.39
23	A	407	CLA	O2D-CGD	3.30	1.41	1.33
23	B	611	CLA	OBD-CAD	3.30	1.27	1.22
23	C	501	CLA	C4B-CHC	3.30	1.48	1.39
23	a	411	CLA	CHB-C4A	3.29	1.37	1.33
23	B	605	CLA	C3B-C2B	3.29	1.44	1.40
36	D	408	LHG	O8-C23	3.29	1.43	1.33
23	B	611	CLA	C4B-CHC	3.29	1.48	1.39
23	A	407	CLA	C3D-C2D	3.28	1.48	1.40
36	D	409	LHG	O8-C23	3.28	1.43	1.33
23	b	604	CLA	C1B-CHB	3.28	1.48	1.39
23	B	603	CLA	C4C-C3C	3.28	1.51	1.45
23	b	618	CLA	CHC-C1C	3.27	1.46	1.35
24	a	413	PHO	C3D-C2D	3.27	1.48	1.40
23	B	616	CLA	CHD-C4C	3.27	1.49	1.41
23	b	611	CLA	O2D-CGD	3.27	1.41	1.33
23	B	617	CLA	C3D-C2D	3.27	1.48	1.40
26	A	412	SQD	O48-C23	3.26	1.43	1.33
23	b	609	CLA	OBD-CAD	3.26	1.27	1.22
34	C	516	DGD	O1G-C1A	3.26	1.43	1.33
23	c	908	CLA	C4B-CHC	3.26	1.48	1.39
23	B	611	CLA	O2D-CGD	3.26	1.41	1.33
23	A	405	CLA	CHD-C4C	3.25	1.49	1.41
23	c	908	CLA	C1B-CHB	3.25	1.48	1.39
23	c	903	CLA	CHC-C1C	3.26	1.46	1.35
23	C	513	CLA	O2A-CGA	3.25	1.43	1.33
23	C	507	CLA	C3D-C2D	3.25	1.47	1.40
23	B	605	CLA	C1B-CHB	3.25	1.48	1.39
34	C	516	DGD	O2G-C1B	3.25	1.44	1.34
24	a	412	PHO	C3D-C2D	3.25	1.47	1.40
23	c	913	CLA	C1B-CHB	3.25	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	F	101	HEM	C3D-C2D	3.24	1.52	1.43
33	b	627	HTG	C1'-S1	-3.24	1.76	1.81
23	b	606	CLA	C1B-C2B	3.24	1.48	1.43
23	C	501	CLA	C3D-C2D	3.24	1.47	1.40
23	c	911	CLA	MG-NA	3.24	2.16	2.07
23	b	605	CLA	O2A-CGA	3.23	1.43	1.33
23	B	610	CLA	C4B-CHC	3.23	1.48	1.39
23	d	403	CLA	OBD-CAD	3.23	1.27	1.22
34	c	917	DGD	O5D-C1E	3.22	1.46	1.40
23	B	615	CLA	C3B-C2B	3.22	1.44	1.40
23	a	411	CLA	OBD-CAD	3.22	1.26	1.22
23	C	507	CLA	OBD-CAD	3.22	1.26	1.22
23	b	613	CLA	C3B-C2B	3.22	1.44	1.40
23	b	616	CLA	C4A-NA	-3.22	1.32	1.38
23	c	910	CLA	CHC-C1C	3.21	1.46	1.35
23	c	903	CLA	O2A-CGA	3.21	1.43	1.33
23	B	615	CLA	O2A-CGA	3.21	1.43	1.33
23	C	504	CLA	C1B-CHB	3.20	1.48	1.39
23	c	902	CLA	C1B-C2B	3.20	1.48	1.43
28	A	414	PL9	C7-C3	3.20	1.54	1.51
23	c	913	CLA	C4C-C3C	3.20	1.50	1.45
23	B	614	CLA	C1B-CHB	3.19	1.48	1.39
23	d	403	CLA	C3D-C2D	3.19	1.47	1.40
23	C	501	CLA	O2D-CGD	3.19	1.41	1.33
23	c	902	CLA	C4C-C3C	3.19	1.50	1.45
23	B	614	CLA	CHB-C4A	3.19	1.37	1.33
23	B	605	CLA	CHC-C1C	3.18	1.45	1.35
36	D	410	LHG	O7-C7	3.18	1.43	1.34
23	B	610	CLA	O2A-CGA	3.18	1.43	1.33
23	a	409	CLA	C4A-NA	-3.17	1.33	1.38
23	c	909	CLA	C1B-C2B	3.17	1.48	1.43
23	c	906	CLA	C1B-CHB	3.17	1.48	1.39
23	a	409	CLA	MG-NB	-3.17	1.98	2.05
23	B	608	CLA	MG-NC	3.17	2.16	2.07
23	b	617	CLA	CHC-C1C	3.16	1.45	1.35
23	B	613	CLA	CHD-C4C	3.16	1.48	1.41
23	D	403	CLA	O2D-CGD	3.16	1.41	1.33
23	d	402	CLA	C4B-CHC	3.16	1.48	1.39
23	b	615	CLA	OBD-CAD	3.16	1.26	1.22
23	b	619	CLA	C3D-C2D	3.16	1.47	1.40
23	c	907	CLA	OBD-CAD	3.15	1.26	1.22
34	h	102	DGD	O1G-C1A	3.16	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	MG-NA	3.15	2.16	2.07
23	B	616	CLA	C4A-NA	-3.15	1.33	1.38
23	C	509	CLA	C3B-C2B	3.15	1.44	1.40
25	a	415	BCR	C26-C25	3.15	1.39	1.34
34	D	406	DGD	CGA-CFA	-3.14	1.53	1.55
23	b	613	CLA	CHB-C4A	3.14	1.37	1.33
27	b	623	LMG	O7-C10	3.14	1.43	1.34
23	B	608	CLA	OBD-CAD	3.13	1.26	1.22
23	B	616	CLA	C3D-C2D	3.13	1.47	1.40
23	A	405	CLA	C1B-CHB	3.13	1.48	1.39
23	A	405	CLA	CHB-C4A	3.13	1.37	1.33
23	b	616	CLA	C1B-C2B	3.13	1.48	1.43
23	C	505	CLA	C3D-C2D	3.12	1.47	1.40
23	B	608	CLA	CHD-C4C	3.12	1.48	1.41
23	b	608	CLA	C1B-C2B	3.12	1.48	1.43
23	B	608	CLA	C4A-NA	-3.12	1.33	1.38
23	A	405	CLA	MG-ND	-3.11	1.98	2.05
23	c	912	CLA	C3D-C2D	3.11	1.47	1.40
34	D	406	DGD	O3G-C1D	3.11	1.45	1.40
23	B	608	CLA	MG-ND	3.11	2.11	2.05
23	C	512	CLA	CHD-C4C	3.11	1.48	1.41
23	C	511	CLA	CHD-C4C	3.11	1.48	1.41
23	c	902	CLA	C4C-NC	-3.10	1.32	1.37
23	c	907	CLA	CHD-C4C	3.10	1.48	1.41
33	d	401	HTG	C1'-S1	-3.10	1.77	1.81
23	C	509	CLA	C3D-C2D	3.10	1.47	1.40
23	C	501	CLA	CHD-C4C	3.10	1.48	1.41
23	b	609	CLA	C1B-CHB	3.10	1.48	1.39
23	c	911	CLA	C1B-CHB	3.09	1.48	1.39
23	D	403	CLA	C3D-C2D	3.10	1.47	1.40
23	c	914	CLA	CHD-C4C	3.09	1.48	1.41
34	h	102	DGD	O2G-C1B	3.09	1.43	1.34
23	b	610	CLA	C3B-C2B	3.09	1.44	1.40
23	B	611	CLA	O2A-CGA	3.09	1.42	1.33
30	J	102	LMT	O1'-C1'	3.09	1.45	1.40
23	c	905	CLA	O2A-CGA	3.09	1.42	1.33
23	b	608	CLA	C1D-ND	-3.09	1.30	1.38
23	B	606	CLA	OBD-CAD	3.08	1.26	1.22
23	b	605	CLA	C1B-CHB	3.09	1.48	1.39
23	c	910	CLA	C3D-C2D	3.09	1.47	1.40
23	C	505	CLA	C4B-CHC	3.08	1.48	1.39
23	C	512	CLA	MG-ND	3.08	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C1B-CHB	3.08	1.48	1.39
23	c	904	CLA	O2A-CGA	3.08	1.42	1.33
23	c	912	CLA	CHD-C4C	3.07	1.48	1.41
24	a	413	PHO	C1D-C2D	3.07	1.49	1.44
23	C	512	CLA	OBD-CAD	3.07	1.26	1.22
38	H	101	RRX	C5-C6	3.07	1.39	1.34
23	C	501	CLA	MG-ND	3.07	2.11	2.05
23	c	907	CLA	CHC-C1C	3.06	1.45	1.35
23	c	904	CLA	C4A-NA	-3.06	1.33	1.38
24	a	413	PHO	C4D-ND	3.06	1.41	1.36
23	C	512	CLA	C4A-NA	-3.05	1.33	1.38
23	A	410	CLA	C4D-C3D	-3.06	1.36	1.42
23	b	619	CLA	C1B-CHB	3.05	1.48	1.39
23	c	909	CLA	O2A-CGA	3.05	1.42	1.33
23	D	403	CLA	C1B-C2B	3.05	1.48	1.43
37	v	201	HEM	C1C-NC	3.05	1.41	1.33
23	b	614	CLA	C3D-C2D	3.05	1.47	1.40
23	b	619	CLA	C4B-CHC	3.04	1.48	1.39
34	C	517	DGD	O2G-C1B	3.04	1.43	1.34
23	B	610	CLA	OBD-CAD	3.04	1.26	1.22
23	C	509	CLA	C4A-NA	-3.03	1.33	1.38
23	b	615	CLA	O2A-CGA	3.03	1.42	1.33
23	C	503	CLA	C4B-CHC	3.03	1.48	1.39
25	a	415	BCR	C8-C9	3.03	1.52	1.45
23	b	612	CLA	C3D-C2D	3.03	1.47	1.40
23	B	603	CLA	C3D-C2D	3.03	1.47	1.40
23	b	611	CLA	C1B-CHB	3.03	1.48	1.39
23	c	904	CLA	C3D-C2D	3.03	1.47	1.40
23	C	507	CLA	C4B-CHC	3.02	1.48	1.39
23	c	905	CLA	C4C-C3C	3.02	1.50	1.45
23	d	403	CLA	C4B-CHC	3.02	1.48	1.39
23	C	511	CLA	C1B-C2B	3.02	1.48	1.43
23	b	604	CLA	CHD-C4C	3.01	1.48	1.41
34	c	917	DGD	O1G-C1A	3.01	1.42	1.33
23	a	410	CLA	O2A-CGA	3.01	1.42	1.33
23	D	402	CLA	C4D-ND	-3.01	1.30	1.38
23	B	606	CLA	O2A-CGA	3.00	1.42	1.33
23	C	501	CLA	O2A-CGA	3.00	1.42	1.33
23	a	411	CLA	MG-NA	3.00	2.16	2.07
23	A	410	CLA	O2A-CGA	3.00	1.42	1.33
23	C	506	CLA	C4B-CHC	2.99	1.48	1.39
28	D	405	PL9	C18-C19	2.99	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	408	PHO	C1A-NA	-2.99	1.30	1.37
23	A	405	CLA	MG-NB	2.98	2.11	2.05
23	B	608	CLA	O2D-CGD	2.98	1.40	1.33
23	C	505	CLA	C4C-C3C	2.98	1.50	1.45
25	D	404	BCR	C5-C6	2.98	1.39	1.34
23	B	614	CLA	C3B-C2B	2.98	1.44	1.40
23	b	617	CLA	C4B-CHC	2.97	1.48	1.39
24	A	409	PHO	C1A-NA	-2.97	1.30	1.37
23	C	507	CLA	C1C-C2C	2.97	1.50	1.44
23	B	616	CLA	C4C-C3C	2.97	1.50	1.45
34	c	919	DGD	O2G-C2G	-2.97	1.39	1.46
23	D	402	CLA	CHC-C1C	2.96	1.45	1.35
23	C	513	CLA	C1B-C2B	2.96	1.48	1.43
23	C	502	CLA	C1B-CHB	2.96	1.48	1.39
23	b	615	CLA	C3D-C2D	2.96	1.47	1.40
36	l	101	LHG	O8-C23	2.96	1.42	1.33
23	c	904	CLA	C4B-CHC	2.95	1.48	1.39
23	B	603	CLA	O2D-CGD	2.95	1.40	1.33
23	C	513	CLA	C4A-NA	-2.95	1.33	1.38
38	H	101	RRX	C33-C5	2.95	1.56	1.51
30	M	101	LMT	O1'-C1'	2.95	1.45	1.40
23	b	612	CLA	C1B-CHB	2.95	1.48	1.39
23	c	914	CLA	C1B-C2B	2.94	1.48	1.43
36	d	407	LHG	O8-C23	2.94	1.42	1.33
23	a	410	CLA	CHD-C4C	2.94	1.48	1.41
23	B	607	CLA	C4C-C3C	2.94	1.50	1.45
30	a	402	LMT	O1'-C1'	2.94	1.45	1.40
27	B	622	LMG	O7-C10	2.93	1.43	1.34
23	C	513	CLA	CHD-C4C	2.93	1.48	1.41
23	b	607	CLA	C1B-CHB	2.93	1.47	1.39
23	c	911	CLA	CHD-C4C	2.93	1.48	1.41
23	B	613	CLA	C1B-CHB	2.93	1.47	1.39
23	c	907	CLA	C1B-C2B	2.92	1.48	1.43
34	c	917	DGD	CGB-CFB	-2.92	1.54	1.55
36	d	409	LHG	O7-C7	2.92	1.43	1.34
23	C	508	CLA	O2A-CGA	2.92	1.42	1.33
23	b	617	CLA	CHD-C4C	2.92	1.48	1.41
23	c	908	CLA	CHD-C4C	2.92	1.48	1.41
23	B	606	CLA	C1B-C2B	2.92	1.48	1.43
23	c	909	CLA	C1B-CHB	2.92	1.47	1.39
23	c	914	CLA	C4B-CHC	2.91	1.47	1.39
23	c	909	CLA	C1C-NC	-2.91	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C1B-C2B	2.91	1.48	1.43
23	b	609	CLA	C3D-C2D	2.90	1.47	1.40
23	C	508	CLA	C4B-CHC	2.90	1.47	1.39
23	C	512	CLA	C4C-C3C	2.90	1.50	1.45
23	b	611	CLA	C1B-C2B	2.90	1.48	1.43
23	C	505	CLA	C1B-CHB	2.90	1.47	1.39
23	C	513	CLA	C4B-CHC	2.89	1.47	1.39
24	A	409	PHO	C3D-C4D	-2.89	1.35	1.40
23	B	612	CLA	C3D-C2D	2.89	1.47	1.40
37	F	101	HEM	C4D-ND	2.89	1.41	1.33
23	D	402	CLA	C1D-ND	-2.88	1.31	1.38
36	d	409	LHG	O8-C23	2.88	1.42	1.33
23	C	502	CLA	O2A-CGA	2.88	1.42	1.33
23	b	604	CLA	C4A-NA	-2.88	1.33	1.38
23	b	619	CLA	C1C-C2C	2.88	1.50	1.44
23	c	906	CLA	MG-NB	2.88	2.11	2.05
23	B	604	CLA	C4A-NA	-2.88	1.33	1.38
23	C	503	CLA	CHD-C4C	2.88	1.48	1.41
23	C	507	CLA	C1B-CHB	2.88	1.47	1.39
23	B	608	CLA	C3D-C2D	2.87	1.47	1.40
23	b	610	CLA	C4A-NA	-2.87	1.33	1.38
23	b	612	CLA	MG-NA	2.87	2.15	2.07
33	c	923	HTG	C1-S1	-2.87	1.76	1.80
23	B	610	CLA	C3D-C2D	2.87	1.47	1.40
23	b	606	CLA	C3D-C2D	2.86	1.47	1.40
33	B	630	HTG	C1-S1	-2.86	1.76	1.80
23	c	905	CLA	C4A-NA	-2.86	1.33	1.38
23	C	508	CLA	CHD-C4C	2.86	1.48	1.41
23	b	605	CLA	MG-NB	2.86	2.11	2.05
23	C	505	CLA	O2A-CGA	2.86	1.42	1.33
23	C	510	CLA	C3D-C2D	2.85	1.47	1.40
23	B	607	CLA	C1B-CHB	2.85	1.47	1.39
23	C	502	CLA	C3D-C2D	2.85	1.47	1.40
23	C	504	CLA	MG-NB	2.85	2.11	2.05
23	b	610	CLA	C1B-CHB	2.84	1.47	1.39
23	c	911	CLA	C4B-CHC	2.84	1.47	1.39
37	V	201	HEM	FE-NB	2.84	2.05	1.95
23	B	609	CLA	CHD-C4C	2.83	1.48	1.41
23	c	913	CLA	MG-ND	-2.83	1.98	2.05
26	D	407	SQD	C6-C5	2.82	1.55	1.52
23	b	606	CLA	CHB-C4A	2.82	1.37	1.33
23	c	906	CLA	O2D-CGD	2.82	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	O2A-CGA	2.82	1.41	1.33
23	B	607	CLA	O2A-CGA	2.82	1.41	1.33
23	c	912	CLA	MG-NC	2.82	2.15	2.07
23	b	613	CLA	C4B-CHC	2.82	1.47	1.39
23	C	507	CLA	CHD-C4C	2.82	1.47	1.41
23	c	909	CLA	C4B-CHC	2.82	1.47	1.39
23	b	613	CLA	CHD-C4C	2.82	1.47	1.41
24	A	408	PHO	C1D-C2D	2.82	1.48	1.44
23	b	611	CLA	C4B-CHC	2.81	1.47	1.39
23	b	609	CLA	C4B-CHC	2.82	1.47	1.39
23	A	410	CLA	MG-NA	2.81	2.15	2.07
23	b	608	CLA	O2A-CGA	2.81	1.41	1.33
23	B	611	CLA	C1B-CHB	2.81	1.47	1.39
23	b	609	CLA	CHD-C4C	2.81	1.47	1.41
34	c	918	DGD	O2G-C1B	2.81	1.42	1.34
23	c	906	CLA	C3D-C2D	2.81	1.46	1.40
23	c	911	CLA	MG-ND	-2.80	1.98	2.05
23	c	911	CLA	C4A-NA	-2.80	1.33	1.38
23	b	606	CLA	C1D-ND	-2.80	1.31	1.38
36	L	101	LHG	O8-C23	2.80	1.41	1.33
37	V	201	HEM	C1B-C2B	2.80	1.47	1.45
23	B	603	CLA	CHD-C4C	2.80	1.47	1.41
24	A	409	PHO	C4D-CHA	2.78	1.49	1.44
23	B	605	CLA	O2A-CGA	2.78	1.41	1.33
23	d	403	CLA	C1B-CHB	2.78	1.47	1.39
23	b	607	CLA	C1B-C2B	2.78	1.48	1.43
23	B	614	CLA	C4C-C3C	2.78	1.50	1.45
23	a	409	CLA	O2A-CGA	2.78	1.41	1.33
33	O	303	HTG	O5-C1	2.78	1.46	1.42
23	C	504	CLA	OBD-CAD	2.77	1.26	1.22
24	a	413	PHO	C1B-C2B	2.77	1.49	1.42
23	D	402	CLA	C4B-CHC	2.77	1.47	1.39
28	d	405	PL9	C43-C44	2.76	1.38	1.32
24	A	409	PHO	O2A-CGA	2.76	1.41	1.33
23	C	506	CLA	C3D-C2D	2.76	1.46	1.40
23	B	603	CLA	MG-NC	2.76	2.15	2.07
23	a	411	CLA	O2A-CGA	2.75	1.41	1.33
23	b	611	CLA	CHD-C4C	2.75	1.47	1.41
23	b	616	CLA	C3D-C2D	2.75	1.46	1.40
23	B	602	CLA	C1D-C2D	2.75	1.49	1.42
23	B	613	CLA	C4B-CHC	2.75	1.47	1.39
23	c	910	CLA	C1B-CHB	2.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C4B-CHC	2.75	1.47	1.39
23	a	414	CLA	MG-NB	-2.74	1.98	2.05
23	c	904	CLA	C4C-C3C	2.74	1.50	1.45
33	B	626	HTG	C1'-S1	-2.74	1.77	1.81
23	B	602	CLA	C1B-CHB	2.73	1.47	1.39
23	b	607	CLA	C3D-C2D	2.73	1.46	1.40
23	B	603	CLA	C4B-CHC	2.73	1.47	1.39
23	B	616	CLA	C4C-NC	-2.73	1.32	1.37
23	c	904	CLA	CHD-C4C	2.72	1.47	1.41
23	C	504	CLA	O2A-CGA	2.73	1.41	1.33
23	b	605	CLA	C1D-ND	-2.72	1.31	1.38
23	c	904	CLA	OBD-CAD	2.72	1.26	1.22
23	B	608	CLA	C4B-CHC	2.72	1.47	1.39
23	b	609	CLA	MG-NB	2.72	2.11	2.05
23	C	504	CLA	C1B-C2B	2.72	1.48	1.43
37	f	101	HEM	C4D-ND	2.72	1.40	1.33
23	c	906	CLA	C4B-CHC	2.72	1.47	1.39
26	f	102	SQD	C6-S	-2.72	1.67	1.77
23	C	501	CLA	C1B-C2B	2.71	1.48	1.43
23	c	905	CLA	C1C-NC	-2.72	1.32	1.37
23	b	616	CLA	C4B-CHC	2.71	1.47	1.39
23	c	903	CLA	CBD-CAD	-2.71	1.44	1.56
23	c	907	CLA	C1C-C2C	2.71	1.50	1.44
37	v	201	HEM	C1D-ND	2.71	1.40	1.33
23	b	617	CLA	OBD-CAD	2.70	1.26	1.22
33	c	924	HTG	C1'-S1	-2.70	1.77	1.81
28	d	405	PL9	C18-C19	2.70	1.38	1.32
23	c	908	CLA	C1C-C2C	2.70	1.50	1.44
24	A	408	PHO	O2D-CGD	2.70	1.40	1.33
23	B	616	CLA	C1B-CHB	2.70	1.47	1.39
23	b	604	CLA	C1C-C2C	2.70	1.50	1.44
23	b	614	CLA	C1B-C2B	2.69	1.48	1.43
23	D	403	CLA	C4C-C3C	2.69	1.50	1.45
23	C	504	CLA	C3D-C2D	2.69	1.46	1.40
23	C	509	CLA	C4C-NC	-2.69	1.32	1.37
23	b	615	CLA	MG-NC	-2.69	1.99	2.07
23	C	506	CLA	CHD-C4C	2.69	1.47	1.41
23	c	904	CLA	C1B-C2B	2.69	1.48	1.43
23	D	402	CLA	C3B-CAB	2.68	1.53	1.47
23	B	612	CLA	O2D-CGD	2.69	1.40	1.33
23	C	509	CLA	C1D-CHD	2.69	1.49	1.37
23	a	409	CLA	CHC-C1C	2.68	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C4D-CHA	2.68	1.50	1.38
23	c	913	CLA	CHD-C4C	2.68	1.47	1.41
23	c	911	CLA	C1B-C2B	2.67	1.48	1.43
23	B	609	CLA	CHC-C1C	2.67	1.44	1.35
23	b	613	CLA	C1B-CHB	2.67	1.47	1.39
23	B	604	CLA	C1C-NC	-2.67	1.32	1.37
23	b	615	CLA	C1B-CHB	2.67	1.47	1.39
23	B	609	CLA	C1B-CHB	2.67	1.47	1.39
23	C	505	CLA	CHD-C4C	2.67	1.47	1.41
23	b	606	CLA	MG-ND	2.67	2.10	2.05
26	B	621	SQD	O6-C1	2.66	1.45	1.40
23	C	510	CLA	CHC-C1C	2.66	1.44	1.35
34	H	102	DGD	O2G-C1B	2.66	1.42	1.34
23	c	906	CLA	C4C-C3C	2.66	1.49	1.45
23	b	609	CLA	C1B-NB	2.66	1.38	1.34
24	A	409	PHO	C3D-C2D	2.66	1.46	1.40
23	c	902	CLA	C4B-CHC	2.65	1.47	1.39
23	b	604	CLA	C4D-CHA	2.65	1.49	1.38
23	A	406	CLA	MG-NA	2.65	2.15	2.07
36	L	101	LHG	O7-C7	2.65	1.42	1.34
27	D	411	LMG	O8-C28	2.64	1.41	1.33
23	b	618	CLA	C4A-NA	-2.64	1.33	1.38
23	a	411	CLA	C1B-C2B	2.64	1.47	1.43
23	D	403	CLA	C1C-NC	-2.64	1.33	1.37
23	A	405	CLA	C3D-C2D	2.64	1.46	1.40
23	c	909	CLA	OBD-CAD	2.64	1.26	1.22
23	c	911	CLA	C3D-C2D	2.63	1.46	1.40
23	B	617	CLA	C4B-CHC	2.63	1.47	1.39
23	B	608	CLA	C1D-C2D	2.63	1.49	1.42
23	B	605	CLA	CHD-C4C	2.62	1.47	1.41
23	b	606	CLA	O2A-CGA	2.62	1.41	1.33
23	b	614	CLA	CHD-C4C	2.62	1.47	1.41
23	B	605	CLA	MG-ND	2.62	2.10	2.05
23	C	505	CLA	C1D-ND	-2.62	1.31	1.38
23	B	609	CLA	MG-NA	2.62	2.15	2.07
23	B	602	CLA	CHD-C4C	2.62	1.47	1.41
23	b	609	CLA	O2A-CGA	2.62	1.41	1.33
23	D	403	CLA	CHD-C4C	2.62	1.47	1.41
23	c	911	CLA	C1A-NA	-2.62	1.26	1.32
23	c	904	CLA	MG-ND	2.62	2.10	2.05
23	b	609	CLA	C4D-CHA	2.62	1.49	1.38
23	a	410	CLA	C1D-C2D	2.61	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	617	CLA	MG-NA	2.61	2.15	2.07
23	B	615	CLA	C3D-C2D	2.61	1.46	1.40
28	d	405	PL9	C41-C39	2.61	1.57	1.51
28	a	419	PL9	C6-C5	2.61	1.50	1.35
23	B	610	CLA	C1D-ND	-2.60	1.31	1.38
23	a	411	CLA	C4D-CHA	2.60	1.49	1.38
23	A	406	CLA	C1D-C2D	2.60	1.49	1.42
23	c	908	CLA	C4D-CHA	2.60	1.49	1.38
33	b	601	HTG	C1'-S1	-2.60	1.77	1.81
23	c	907	CLA	C1B-CHB	2.59	1.47	1.39
23	B	611	CLA	C1C-NC	-2.59	1.33	1.37
23	C	503	CLA	CHB-C4A	2.59	1.36	1.33
36	D	409	LHG	O7-C7	2.59	1.42	1.34
23	c	906	CLA	C4A-NA	-2.59	1.34	1.38
23	c	912	CLA	C1D-CHD	2.59	1.49	1.37
34	D	406	DGD	CGB-CFB	-2.58	1.54	1.55
23	b	604	CLA	C4C-C3C	2.58	1.49	1.45
23	B	603	CLA	C1D-C2D	2.58	1.49	1.42
23	C	507	CLA	C1B-C2B	2.58	1.47	1.43
23	c	912	CLA	CHB-C4A	2.58	1.36	1.33
23	b	619	CLA	C1D-ND	-2.58	1.31	1.38
27	d	410	LMG	O7-C8	-2.58	1.40	1.46
28	d	405	PL9	C6-C5	2.58	1.50	1.35
34	c	918	DGD	O2G-C2G	-2.57	1.40	1.46
23	b	607	CLA	MG-NC	2.57	2.14	2.07
23	b	612	CLA	C4C-C3C	2.57	1.49	1.45
23	b	609	CLA	MG-ND	2.57	2.10	2.05
23	A	410	CLA	C4C-C3C	2.57	1.49	1.45
23	C	509	CLA	C1B-CHB	2.57	1.46	1.39
23	C	511	CLA	C4D-CHA	2.56	1.49	1.38
24	a	412	PHO	C1A-NA	-2.56	1.31	1.37
23	b	610	CLA	O2A-CGA	2.56	1.41	1.33
23	B	614	CLA	O2A-CGA	2.56	1.41	1.33
28	D	405	PL9	C22-C23	2.56	1.58	1.50
30	B	623	LMT	O1'-C1'	2.56	1.44	1.40
23	c	902	CLA	CHD-C4C	2.56	1.47	1.41
23	B	609	CLA	C3D-C2D	2.56	1.46	1.40
23	B	617	CLA	C1B-CHB	2.56	1.46	1.39
37	F	101	HEM	FE-NA	2.56	2.14	1.94
34	c	919	DGD	O2G-C1B	2.55	1.42	1.34
28	A	414	PL9	C2-C3	2.55	1.41	1.34
23	C	509	CLA	C4B-CHC	2.55	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	O2A-CGA	2.55	1.41	1.33
23	C	501	CLA	C1B-CHB	2.55	1.46	1.39
23	B	612	CLA	CBD-CAD	-2.55	1.44	1.56
30	Z	102	LMT	O1'-C1'	2.55	1.44	1.40
23	B	607	CLA	C3D-C2D	2.55	1.46	1.40
23	d	403	CLA	CHD-C4C	2.54	1.47	1.41
23	C	511	CLA	MG-NB	-2.54	1.99	2.05
23	c	914	CLA	C1C-C2C	2.54	1.49	1.44
23	b	618	CLA	O2A-CGA	2.54	1.41	1.33
23	c	911	CLA	C4C-NC	-2.53	1.33	1.37
23	b	612	CLA	C1D-C2D	2.53	1.49	1.42
33	C	522	HTG	C1'-S1	-2.53	1.77	1.81
23	B	617	CLA	C2-C3	2.53	1.38	1.32
23	B	610	CLA	C1B-CHB	2.53	1.46	1.39
23	C	502	CLA	C4B-CHC	2.53	1.46	1.39
23	b	607	CLA	MG-NB	2.53	2.10	2.05
37	V	201	HEM	C4A-NA	2.53	1.40	1.36
23	b	617	CLA	MG-ND	-2.52	1.99	2.05
23	D	402	CLA	CHD-C4C	2.52	1.47	1.41
23	a	411	CLA	C1B-CHB	2.52	1.46	1.39
23	b	605	CLA	C4C-C3C	2.52	1.49	1.45
23	B	611	CLA	C1D-CHD	2.52	1.48	1.37
23	B	609	CLA	OBD-CAD	2.52	1.25	1.22
33	c	923	HTG	C1'-S1	-2.52	1.77	1.81
23	b	610	CLA	C4B-CHC	2.52	1.46	1.39
28	A	414	PL9	C6-C5	2.51	1.50	1.35
23	c	904	CLA	C4D-CHA	2.51	1.49	1.38
25	b	622	BCR	C26-C25	2.51	1.38	1.34
23	b	607	CLA	C1D-C2D	2.51	1.48	1.42
23	c	909	CLA	C1C-C2C	2.51	1.49	1.44
23	D	403	CLA	C4C-NC	-2.50	1.33	1.37
23	a	414	CLA	CHD-C4C	2.50	1.47	1.41
23	C	507	CLA	C4C-C3C	2.50	1.49	1.45
23	C	509	CLA	C4C-C3C	2.50	1.49	1.45
23	B	602	CLA	C4D-CHA	2.50	1.49	1.38
37	F	101	HEM	C1D-ND	2.50	1.40	1.33
23	b	612	CLA	C4B-CHC	2.50	1.46	1.39
23	B	604	CLA	C1D-CHD	2.49	1.48	1.37
23	b	615	CLA	C4B-CHC	2.49	1.46	1.39
23	B	614	CLA	O2D-CGD	2.49	1.39	1.33
24	a	413	PHO	OBD-CAD	2.49	1.25	1.22
37	v	201	HEM	C1A-C2A	2.49	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C1D-C2D	2.49	1.48	1.42
24	a	413	PHO	C4B-C3B	2.49	1.48	1.42
23	d	403	CLA	C1D-C2D	2.49	1.48	1.42
23	B	602	CLA	C3D-C2D	2.48	1.46	1.40
23	A	407	CLA	O2A-CGA	2.48	1.40	1.33
23	d	402	CLA	C1D-CHD	2.48	1.48	1.37
23	B	612	CLA	C4B-CHC	2.48	1.46	1.39
23	b	611	CLA	C3D-C2D	2.47	1.46	1.40
23	C	505	CLA	C1D-CHD	2.48	1.48	1.37
25	B	619	BCR	C5-C6	2.47	1.38	1.34
25	t	101	BCR	C23-C22	2.47	1.51	1.45
30	b	624	LMT	O1'-C1'	2.47	1.44	1.40
23	B	617	CLA	C1B-C2B	2.47	1.47	1.43
23	D	402	CLA	MG-ND	2.47	2.10	2.05
23	c	910	CLA	MG-NC	2.47	2.14	2.07
23	C	503	CLA	C1C-C2C	2.47	1.49	1.44
23	b	609	CLA	C4A-NA	-2.47	1.34	1.38
36	d	408	LHG	O7-C7	2.47	1.41	1.34
23	b	606	CLA	C1B-CHB	2.46	1.46	1.39
23	B	611	CLA	MG-NC	2.46	2.14	2.07
23	a	410	CLA	C1B-CHB	2.46	1.46	1.39
28	D	405	PL9	C6-C5	2.46	1.49	1.35
23	A	405	CLA	C4A-NA	-2.46	1.34	1.38
38	H	101	RRX	C1-C6	2.46	1.57	1.53
36	l	101	LHG	O7-C7	2.46	1.41	1.34
23	C	512	CLA	C4D-CHA	2.45	1.49	1.38
36	d	408	LHG	O8-C23	2.45	1.40	1.33
23	c	914	CLA	C1D-CHD	2.45	1.48	1.37
23	B	606	CLA	C3D-C2D	2.45	1.46	1.40
30	c	922	LMT	O1'-C1'	2.45	1.44	1.40
23	C	503	CLA	MG-ND	2.44	2.10	2.05
23	A	406	CLA	C1D-ND	-2.44	1.32	1.38
28	d	405	PL9	C13-C14	2.44	1.37	1.32
23	c	912	CLA	C4D-CHA	2.44	1.48	1.38
23	A	410	CLA	C3D-C2D	2.44	1.46	1.40
23	a	411	CLA	C4C-NC	-2.44	1.33	1.37
23	b	605	CLA	C3D-C2D	2.44	1.46	1.40
23	C	501	CLA	C4D-CHA	2.44	1.48	1.38
26	L	103	SQD	C6-C5	2.43	1.54	1.52
23	c	909	CLA	C4C-NC	-2.44	1.33	1.37
23	b	608	CLA	MG-NB	2.43	2.10	2.05
23	C	503	CLA	CBD-CAD	-2.43	1.45	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C1D-C2D	2.43	1.48	1.42
23	C	503	CLA	C4C-C3C	2.43	1.49	1.45
23	B	602	CLA	MG-ND	-2.43	1.99	2.05
23	a	414	CLA	C1D-C2D	2.43	1.48	1.42
23	B	604	CLA	CHB-C4A	2.43	1.36	1.33
23	C	510	CLA	C1C-NC	-2.42	1.33	1.37
23	B	611	CLA	C1B-C2B	2.42	1.47	1.43
23	D	402	CLA	C1A-NA	2.42	1.37	1.32
24	a	413	PHO	C4C-C3C	2.42	1.49	1.45
23	c	903	CLA	C4B-CHC	2.42	1.46	1.39
23	c	907	CLA	C3D-C2D	2.42	1.45	1.40
23	a	411	CLA	C4C-C3C	2.41	1.49	1.45
23	C	503	CLA	C3D-C2D	2.42	1.45	1.40
28	D	405	PL9	C28-C29	2.41	1.37	1.32
23	c	905	CLA	C4B-CHC	2.41	1.46	1.39
23	B	613	CLA	C4B-NB	-2.41	1.30	1.34
24	A	408	PHO	C3D-C4D	-2.41	1.36	1.40
37	v	201	HEM	C4D-ND	2.41	1.39	1.33
23	B	610	CLA	C2-C3	2.41	1.37	1.32
33	B	630	HTG	C1'-S1	-2.41	1.78	1.81
23	B	604	CLA	MG-NB	-2.41	1.99	2.05
23	a	414	CLA	CHB-C4A	2.41	1.36	1.33
23	d	403	CLA	MG-ND	2.40	2.10	2.05
23	B	613	CLA	C3D-C2D	2.40	1.45	1.40
23	B	614	CLA	CHD-C4C	2.40	1.46	1.41
23	b	613	CLA	MG-NC	2.40	2.14	2.07
23	b	614	CLA	C4D-CHA	2.40	1.48	1.38
23	c	909	CLA	C1D-CHD	2.40	1.48	1.37
23	D	403	CLA	C4A-NA	-2.40	1.34	1.38
23	C	509	CLA	C1B-C2B	2.40	1.47	1.43
23	C	512	CLA	C4B-CHC	2.39	1.46	1.39
33	C	521	HTG	C1'-S1	-2.39	1.78	1.81
23	C	510	CLA	CHD-C4C	2.39	1.46	1.41
26	B	621	SQD	C6-C5	2.39	1.54	1.52
33	b	601	HTG	C1-S1	-2.39	1.76	1.80
23	b	612	CLA	C1D-CHD	2.39	1.48	1.37
23	A	410	CLA	CBD-CAD	-2.39	1.45	1.56
23	B	616	CLA	C1D-C2D	2.39	1.48	1.42
23	b	606	CLA	C4D-CHA	2.39	1.48	1.38
23	B	604	CLA	CHD-C4C	2.38	1.46	1.41
23	b	614	CLA	C1D-CHD	2.38	1.48	1.37
23	b	618	CLA	C1B-CHB	2.38	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	620	BCR	C23-C22	2.38	1.51	1.45
23	B	604	CLA	C2-C3	2.38	1.37	1.32
23	b	613	CLA	O2A-CGA	2.37	1.40	1.33
23	b	613	CLA	C3D-C2D	2.38	1.45	1.40
23	b	619	CLA	C1B-C2B	2.37	1.47	1.43
33	b	627	HTG	C1-S1	-2.37	1.76	1.80
23	d	403	CLA	C1B-C2B	2.37	1.47	1.43
23	B	607	CLA	C4B-CHC	2.37	1.46	1.39
25	a	415	BCR	C27-C26	2.37	1.56	1.51
23	c	911	CLA	CBD-CAD	-2.37	1.45	1.56
23	b	616	CLA	C4C-C3C	2.37	1.49	1.45
23	b	609	CLA	C1C-C2C	2.36	1.49	1.44
25	D	404	BCR	C30-C25	-2.37	1.50	1.53
23	C	501	CLA	C1D-C2D	2.37	1.48	1.42
23	c	910	CLA	C4B-CHC	2.36	1.46	1.39
23	C	510	CLA	C4C-C3C	2.36	1.49	1.45
23	B	614	CLA	C1C-NC	-2.36	1.33	1.37
23	C	504	CLA	C1C-NC	-2.36	1.33	1.37
23	C	508	CLA	C1A-NA	-2.36	1.27	1.32
23	a	409	CLA	CHD-C4C	2.35	1.46	1.41
23	a	410	CLA	CHB-C4A	2.35	1.36	1.33
23	A	406	CLA	C4A-NA	-2.35	1.34	1.38
23	a	409	CLA	C4D-CHA	2.35	1.48	1.38
23	c	914	CLA	C4D-CHA	2.35	1.48	1.38
23	B	603	CLA	C4B-NB	2.35	1.38	1.34
23	C	508	CLA	OBD-CAD	2.35	1.25	1.22
23	c	902	CLA	C4D-CHA	2.35	1.48	1.38
23	a	411	CLA	C4B-CHC	2.34	1.46	1.39
23	B	611	CLA	C4D-CHA	2.34	1.48	1.38
23	c	909	CLA	C4A-NA	-2.34	1.34	1.38
23	a	410	CLA	O2D-CGD	2.34	1.39	1.33
23	c	905	CLA	C1B-C2B	2.34	1.47	1.43
23	b	618	CLA	C4D-CHA	2.34	1.48	1.38
25	B	618	BCR	C5-C6	2.34	1.38	1.34
23	b	611	CLA	C4D-CHA	2.34	1.48	1.38
23	a	409	CLA	C1D-C2D	2.34	1.48	1.42
23	B	615	CLA	C1A-NA	-2.34	1.27	1.32
23	b	610	CLA	C4D-CHA	2.33	1.48	1.38
28	a	419	PL9	C2-C3	2.33	1.41	1.34
23	C	503	CLA	C1D-C2D	2.33	1.48	1.42
23	C	509	CLA	C4D-CHA	2.33	1.48	1.38
23	C	508	CLA	C4C-NC	-2.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	913	CLA	C1D-CHD	2.33	1.48	1.37
23	B	605	CLA	C4C-NC	-2.33	1.33	1.37
23	B	617	CLA	C4C-C3C	2.33	1.49	1.45
23	C	513	CLA	C4D-CHA	2.32	1.48	1.38
23	B	617	CLA	MG-ND	2.32	2.10	2.05
23	B	612	CLA	CHD-C4C	2.32	1.46	1.41
36	d	409	LHG	C4-C5	2.32	1.57	1.50
25	D	404	BCR	C12-C13	2.32	1.51	1.45
23	c	914	CLA	C4C-C3C	2.32	1.49	1.45
34	C	518	DGD	O2G-C1B	2.32	1.41	1.34
23	C	507	CLA	C1D-CHD	2.32	1.48	1.37
23	C	503	CLA	C1B-CHB	2.31	1.46	1.39
23	B	607	CLA	CHD-C4C	2.31	1.46	1.41
33	O	303	HTG	C1'-S1	-2.31	1.78	1.81
23	A	410	CLA	CHD-C4C	2.31	1.46	1.41
23	c	903	CLA	C1B-C2B	2.31	1.47	1.43
23	C	504	CLA	C4D-CHA	2.31	1.48	1.38
34	c	918	DGD	O5D-C1E	2.31	1.44	1.40
24	a	412	PHO	CMA-C3A	2.31	1.58	1.53
23	D	403	CLA	C4B-CHC	2.31	1.46	1.39
23	B	612	CLA	C4C-C3C	2.31	1.49	1.45
23	a	410	CLA	C1-C2	2.31	1.56	1.49
37	v	201	HEM	FE-NB	2.31	2.03	1.95
23	B	602	CLA	MG-NC	2.31	2.14	2.07
23	B	603	CLA	C1D-CHD	2.30	1.48	1.37
23	B	608	CLA	C4C-C3C	2.30	1.49	1.45
23	D	403	CLA	CHB-C4A	2.30	1.36	1.33
34	c	919	DGD	O5D-C1E	2.30	1.44	1.40
23	c	911	CLA	C4D-CHA	2.30	1.48	1.38
34	c	919	DGD	O4D-C4D	2.30	1.48	1.43
23	C	505	CLA	C2A-C1A	-2.30	1.48	1.52
23	b	604	CLA	MG-NB	-2.30	1.99	2.05
23	b	609	CLA	C1B-C2B	2.30	1.47	1.43
23	A	406	CLA	O2D-CGD	2.30	1.39	1.33
23	d	402	CLA	C1D-C2D	2.29	1.48	1.42
36	d	407	LHG	O7-C7	2.29	1.41	1.34
23	b	607	CLA	OBD-CAD	2.29	1.25	1.22
23	B	602	CLA	C4C-C3C	2.29	1.49	1.45
37	V	201	HEM	C1C-NC	2.29	1.39	1.33
23	B	615	CLA	C1D-CHD	2.29	1.47	1.37
23	c	903	CLA	C4D-CHA	2.29	1.48	1.38
23	c	903	CLA	C3D-C2D	2.29	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	913	CLA	C4D-CHA	2.29	1.48	1.38
23	b	606	CLA	CHD-C4C	2.29	1.46	1.41
23	C	502	CLA	C4D-CHA	2.28	1.48	1.38
37	F	101	HEM	CHC-C4B	-2.28	1.37	1.39
23	B	611	CLA	C4C-C3C	2.28	1.49	1.45
23	B	603	CLA	C3B-CAB	2.28	1.52	1.47
25	d	404	BCR	C12-C13	2.28	1.51	1.45
23	A	407	CLA	C3B-C2B	2.28	1.43	1.40
23	b	612	CLA	C4D-CHA	2.28	1.48	1.38
23	b	612	CLA	MG-ND	2.27	2.10	2.05
23	B	602	CLA	C1B-C2B	2.27	1.47	1.43
34	d	406	DGD	O3G-C1D	2.27	1.44	1.40
23	a	414	CLA	MG-ND	2.27	2.10	2.05
25	C	515	BCR	C1-C6	-2.27	1.50	1.53
33	b	626	HTG	C1'-S1	-2.27	1.78	1.81
33	C	522	HTG	O5-C1	2.27	1.45	1.42
23	C	510	CLA	C4D-CHA	2.27	1.48	1.38
23	b	615	CLA	C3B-C2B	2.27	1.43	1.40
28	d	405	PL9	C17-C18	2.26	1.57	1.50
23	B	605	CLA	C1D-CHD	2.26	1.47	1.37
23	b	614	CLA	C4A-NA	-2.26	1.34	1.38
25	b	620	BCR	C23-C22	2.26	1.50	1.45
23	C	508	CLA	C1C-NC	-2.26	1.33	1.37
23	c	905	CLA	C4D-CHA	2.26	1.48	1.38
23	b	612	CLA	CHD-C4C	2.26	1.46	1.41
23	B	613	CLA	O2A-CGA	2.26	1.40	1.33
23	C	503	CLA	C4D-CHA	2.25	1.48	1.38
23	b	619	CLA	C1C-NC	-2.25	1.33	1.37
23	c	903	CLA	C4C-C3C	2.25	1.49	1.45
23	b	613	CLA	C1D-CHD	2.25	1.47	1.37
23	c	902	CLA	C3D-C2D	2.25	1.45	1.40
23	B	602	CLA	C1C-C2C	2.24	1.49	1.44
23	B	617	CLA	MG-NB	2.24	2.10	2.05
23	c	903	CLA	C4C-NC	-2.24	1.33	1.37
23	b	619	CLA	C4D-CHA	2.24	1.48	1.38
23	C	510	CLA	C4B-CHC	2.24	1.46	1.39
28	D	405	PL9	C41-C39	2.24	1.56	1.51
23	b	617	CLA	C1D-CHD	2.24	1.47	1.37
23	C	505	CLA	MG-ND	2.23	2.10	2.05
23	C	506	CLA	C4D-CHA	2.23	1.48	1.38
23	c	906	CLA	C4D-CHA	2.23	1.48	1.38
23	b	604	CLA	C1D-CHD	2.23	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	625	HTG	C1'-S1	-2.23	1.78	1.81
23	b	611	CLA	C4A-NA	-2.22	1.34	1.38
23	A	406	CLA	C4C-C3C	2.22	1.49	1.45
23	B	614	CLA	C4D-CHA	2.22	1.48	1.38
23	B	612	CLA	O2A-CGA	2.22	1.40	1.33
23	C	512	CLA	C1D-CHD	2.22	1.47	1.37
23	C	511	CLA	C4B-CHC	2.22	1.46	1.39
23	C	502	CLA	C1C-NC	-2.22	1.33	1.37
23	a	411	CLA	CHD-C4C	2.22	1.46	1.41
23	C	511	CLA	C4C-NC	-2.22	1.33	1.37
27	C	519	LMG	O7-C8	-2.22	1.41	1.46
37	f	101	HEM	C1C-NC	2.21	1.39	1.33
23	C	511	CLA	CBD-CAD	-2.21	1.46	1.56
25	b	621	BCR	C26-C25	2.21	1.37	1.34
23	A	406	CLA	C3D-C2D	2.21	1.45	1.40
23	a	409	CLA	C1B-CHB	2.21	1.45	1.39
23	A	410	CLA	C1D-CHD	2.21	1.47	1.37
25	k	101	BCR	C26-C25	2.21	1.37	1.34
23	C	513	CLA	C1D-CHD	2.20	1.47	1.37
23	A	410	CLA	MG-NC	2.21	2.13	2.07
23	B	602	CLA	C2-C3	2.21	1.37	1.32
23	c	909	CLA	C1A-NA	-2.20	1.27	1.32
25	d	404	BCR	C33-C5	2.20	1.54	1.51
23	B	617	CLA	C4D-CHA	2.20	1.47	1.38
23	a	410	CLA	MG-ND	-2.20	2.00	2.05
23	a	410	CLA	C4B-CHC	2.20	1.45	1.39
23	b	607	CLA	CHD-C4C	2.20	1.46	1.41
23	c	907	CLA	C4B-CHC	2.20	1.45	1.39
23	b	610	CLA	OBD-CAD	2.20	1.25	1.22
27	c	920	LMG	O3-C3	2.19	1.48	1.43
37	f	101	HEM	C1D-ND	2.19	1.39	1.33
23	b	605	CLA	C4B-CHC	2.19	1.45	1.39
23	a	409	CLA	C1A-NA	-2.19	1.27	1.32
23	b	618	CLA	C4C-C3C	2.19	1.49	1.45
23	B	614	CLA	OBD-CAD	2.19	1.25	1.22
23	a	414	CLA	CBD-CAD	-2.18	1.46	1.56
23	A	407	CLA	C4D-CHA	2.18	1.47	1.38
23	D	402	CLA	C4D-CHA	2.18	1.47	1.38
23	b	605	CLA	C4A-NA	-2.18	1.34	1.38
23	c	914	CLA	C4A-NA	-2.17	1.34	1.38
25	k	102	BCR	C26-C25	2.17	1.37	1.34
23	c	904	CLA	C1D-CHD	2.17	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C1B-CHB	2.17	1.45	1.39
37	V	201	HEM	C1D-ND	2.17	1.39	1.33
23	d	402	CLA	O2D-CGD	2.17	1.38	1.33
23	B	616	CLA	C4B-CHC	2.17	1.45	1.39
37	V	201	HEM	C3D-C2D	2.17	1.49	1.43
25	c	916	BCR	C12-C13	2.17	1.50	1.45
23	A	407	CLA	C4C-NC	-2.17	1.33	1.37
23	C	513	CLA	MG-ND	-2.16	2.00	2.05
23	C	508	CLA	C1C-C2C	2.16	1.48	1.44
23	b	616	CLA	C4D-CHA	2.16	1.47	1.38
23	c	906	CLA	C1D-CHD	2.16	1.47	1.37
23	c	904	CLA	C1A-NA	-2.16	1.27	1.32
23	B	617	CLA	C1D-ND	-2.16	1.32	1.38
23	c	903	CLA	CHD-C4C	2.16	1.46	1.41
27	Z	101	LMG	O1-C1	2.16	1.44	1.40
23	c	908	CLA	C4C-C3C	2.16	1.49	1.45
23	C	511	CLA	C1B-NB	2.16	1.38	1.34
23	c	910	CLA	C4C-C3C	2.16	1.49	1.45
23	c	910	CLA	C1C-C2C	2.16	1.48	1.44
23	C	510	CLA	C1D-CHD	2.16	1.47	1.37
23	c	909	CLA	C1D-C2D	2.15	1.48	1.42
33	B	631	HTG	O5-C1	2.15	1.45	1.42
23	C	501	CLA	C1D-CHD	2.15	1.47	1.37
23	d	403	CLA	C1D-CHD	2.15	1.47	1.37
23	B	609	CLA	C4D-CHA	2.15	1.47	1.38
23	a	411	CLA	C1D-C2D	2.14	1.48	1.42
23	b	613	CLA	C4D-CHA	2.15	1.47	1.38
23	c	903	CLA	C1C-NC	-2.15	1.33	1.37
23	C	512	CLA	C1C-C2C	2.14	1.48	1.44
28	D	405	PL9	C23-C24	2.14	1.37	1.32
25	B	618	BCR	C30-C25	2.14	1.56	1.53
23	B	605	CLA	C4B-CHC	2.14	1.45	1.39
34	C	516	DGD	O5D-C1E	2.14	1.44	1.40
23	B	613	CLA	C4C-C3C	2.14	1.48	1.45
23	B	610	CLA	O2D-CGD	2.14	1.38	1.33
23	C	509	CLA	MG-ND	2.14	2.09	2.05
23	c	912	CLA	CBD-CAD	-2.13	1.46	1.56
23	b	607	CLA	O2A-CGA	2.13	1.39	1.33
24	a	412	PHO	C2-C3	2.13	1.37	1.32
23	B	612	CLA	C4D-CHA	2.13	1.47	1.38
23	b	609	CLA	C1D-C2D	2.13	1.48	1.42
23	b	614	CLA	OBD-CAD	2.13	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	617	CLA	CHD-C4C	2.13	1.46	1.41
23	C	501	CLA	C1C-C2C	2.13	1.48	1.44
23	b	610	CLA	C1D-CHD	2.13	1.47	1.37
23	b	609	CLA	C1C-NC	-2.13	1.33	1.37
27	c	921	LMG	O1-C1	2.12	1.44	1.40
23	d	402	CLA	OBD-CAD	2.12	1.25	1.22
23	C	508	CLA	C1D-CHD	2.12	1.47	1.37
28	d	405	PL9	C21-C19	2.12	1.56	1.51
37	v	201	HEM	CAA-C2A	2.13	1.55	1.52
23	b	605	CLA	CBD-CAD	-2.12	1.46	1.56
28	D	405	PL9	C13-C14	2.12	1.37	1.32
23	c	904	CLA	MG-NB	2.12	2.09	2.05
23	B	613	CLA	C1D-C2D	2.12	1.47	1.42
23	c	910	CLA	C1C-NC	-2.12	1.33	1.37
23	B	609	CLA	C1D-CHD	2.12	1.47	1.37
23	c	912	CLA	C4C-C3C	2.12	1.48	1.45
37	v	201	HEM	C1A-NA	2.12	1.39	1.36
23	B	603	CLA	CBD-CAD	-2.11	1.46	1.56
23	a	411	CLA	CBD-CAD	-2.11	1.46	1.56
23	B	606	CLA	C4D-CHA	2.11	1.47	1.38
25	K	102	BCR	C12-C13	2.11	1.50	1.45
23	c	911	CLA	MG-NB	-2.11	2.00	2.05
23	c	910	CLA	C1D-CHD	2.11	1.47	1.37
23	a	409	CLA	C3D-C2D	2.11	1.45	1.40
23	a	414	CLA	C1D-ND	-2.11	1.32	1.38
23	c	906	CLA	CHB-C4A	2.11	1.36	1.33
23	B	611	CLA	CHD-C4C	2.11	1.46	1.41
23	b	609	CLA	C1D-CHD	2.11	1.47	1.37
27	c	920	LMG	O1-C1	2.11	1.43	1.40
23	B	612	CLA	C1D-C2D	2.11	1.47	1.42
23	c	907	CLA	C1C-NC	-2.11	1.33	1.37
23	c	914	CLA	C1D-C2D	2.10	1.47	1.42
23	C	511	CLA	MG-ND	2.10	2.09	2.05
30	m	102	LMT	O1'-C1'	2.11	1.43	1.40
23	B	612	CLA	C3B-C2B	2.10	1.43	1.40
23	B	605	CLA	CHB-C4A	2.10	1.36	1.33
23	b	619	CLA	C2-C3	2.10	1.37	1.32
23	b	610	CLA	CHD-C4C	2.10	1.46	1.41
34	h	102	DGD	CGA-CFA	-2.10	1.54	1.55
25	b	620	BCR	C26-C25	2.10	1.37	1.34
23	C	511	CLA	C4C-C3C	2.10	1.48	1.45
23	A	406	CLA	C1-C2	2.10	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C1D-CHD	2.10	1.47	1.37
37	F	101	HEM	CMA-C3A	2.10	1.56	1.51
23	c	910	CLA	C4D-CHA	2.09	1.47	1.38
23	d	403	CLA	C1C-C2C	2.09	1.48	1.44
23	B	607	CLA	C1B-C2B	2.09	1.47	1.43
23	A	410	CLA	C1B-C2B	2.09	1.47	1.43
37	V	201	HEM	C3C-C4C	-2.09	1.43	1.45
23	b	607	CLA	C4D-CHA	2.09	1.47	1.38
23	b	611	CLA	CAA-C2A	2.09	1.57	1.54
23	c	902	CLA	C1D-CHD	2.09	1.47	1.37
23	B	605	CLA	C1D-C2D	2.09	1.47	1.42
25	c	915	BCR	C12-C13	2.08	1.50	1.45
23	C	503	CLA	OBD-CAD	2.09	1.25	1.22
23	B	608	CLA	C1D-CHD	2.09	1.47	1.37
23	D	403	CLA	C4D-C3D	-2.09	1.38	1.42
23	b	610	CLA	C1D-ND	-2.09	1.33	1.38
23	C	501	CLA	C4A-NA	-2.09	1.34	1.38
23	A	405	CLA	C4C-C3C	2.08	1.48	1.45
23	c	908	CLA	C1A-CHA	2.08	1.52	1.43
23	A	407	CLA	C1D-C2D	2.08	1.47	1.42
23	b	617	CLA	C1A-NA	-2.08	1.27	1.32
23	B	608	CLA	C2-C3	2.08	1.37	1.32
23	c	903	CLA	C1D-CHD	2.08	1.47	1.37
23	A	406	CLA	C4D-CHA	2.08	1.47	1.38
23	C	501	CLA	C4C-C3C	2.08	1.48	1.45
25	k	102	BCR	C12-C13	2.08	1.50	1.45
33	B	631	HTG	C1'-S1	-2.08	1.78	1.81
23	b	606	CLA	MG-NC	-2.08	2.01	2.07
23	c	904	CLA	C1C-C2C	2.07	1.48	1.44
23	B	613	CLA	C1D-ND	-2.07	1.33	1.38
23	B	617	CLA	CHB-C4A	2.07	1.36	1.33
23	C	508	CLA	C4D-CHA	2.07	1.47	1.38
33	B	625	HTG	O5-C1	2.07	1.45	1.42
24	A	409	PHO	C1B-C2B	2.07	1.47	1.42
23	B	610	CLA	C4D-CHA	2.07	1.47	1.38
23	C	508	CLA	MG-ND	-2.06	2.00	2.05
23	a	411	CLA	C4D-ND	-2.06	1.33	1.38
23	c	910	CLA	MG-NB	-2.06	2.00	2.05
25	B	619	BCR	C24-C25	2.06	1.53	1.45
25	B	619	BCR	C23-C22	2.06	1.50	1.45
23	B	616	CLA	C1D-CHD	2.05	1.46	1.37
23	C	510	CLA	C4D-C3D	-2.05	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	902	CLA	C1D-C2D	2.05	1.47	1.42
28	D	405	PL9	C12-C13	2.05	1.56	1.50
23	B	604	CLA	CBD-CAD	-2.05	1.47	1.56
23	D	403	CLA	C1D-CHD	2.05	1.46	1.37
23	D	403	CLA	C1B-NB	2.05	1.37	1.34
23	B	610	CLA	MG-NC	2.05	2.13	2.07
23	C	506	CLA	C1C-C2C	2.05	1.48	1.44
23	C	501	CLA	CHB-C4A	2.04	1.36	1.33
23	b	617	CLA	C4C-C3C	2.04	1.48	1.45
23	A	406	CLA	CHD-C4C	2.04	1.46	1.41
23	C	511	CLA	C1C-NC	-2.04	1.34	1.37
23	b	619	CLA	C1D-CHD	2.04	1.46	1.37
30	C	520	LMT	O1'-C1'	2.04	1.43	1.40
23	b	612	CLA	C1A-NA	-2.04	1.27	1.32
23	B	603	CLA	C1D-ND	-2.04	1.33	1.38
23	c	911	CLA	C1D-C2D	2.04	1.47	1.42
23	A	407	CLA	C1D-CHD	2.04	1.46	1.37
33	d	401	HTG	C1-S1	-2.03	1.77	1.80
23	B	613	CLA	C4A-NA	-2.03	1.34	1.38
25	d	404	BCR	C23-C22	2.03	1.50	1.45
23	A	410	CLA	O2D-CGD	2.03	1.38	1.33
23	C	507	CLA	C1A-CHA	2.03	1.51	1.43
23	b	619	CLA	CHD-C4C	2.03	1.46	1.41
23	b	607	CLA	C1C-NC	-2.03	1.34	1.37
23	C	513	CLA	C4C-NC	-2.03	1.34	1.37
23	D	402	CLA	C1B-CHB	2.03	1.45	1.39
36	D	410	LHG	C4-C5	2.03	1.56	1.50
23	B	611	CLA	C4D-C3D	-2.03	1.38	1.42
25	b	621	BCR	C24-C25	2.03	1.53	1.45
23	b	605	CLA	C1D-CHD	2.03	1.46	1.37
23	c	902	CLA	MG-NB	-2.03	2.00	2.05
37	v	201	HEM	FE-NC	2.03	2.03	1.95
33	V	202	HTG	O5-C1	2.02	1.45	1.42
23	A	407	CLA	CHD-C4C	2.02	1.46	1.41
23	B	605	CLA	C3D-C2D	2.02	1.45	1.40
23	C	502	CLA	CHD-C4C	2.02	1.46	1.41
23	a	410	CLA	C1D-CHD	2.02	1.46	1.37
23	b	604	CLA	C1D-C2D	2.02	1.47	1.42
23	b	618	CLA	C1D-C2D	2.02	1.47	1.42
28	D	405	PL9	C2-C1	-2.01	1.38	1.44
23	b	605	CLA	C4D-CHA	2.01	1.47	1.38
23	C	502	CLA	C1D-CHD	2.02	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	905	CLA	C1D-CHD	2.02	1.46	1.37
34	C	518	DGD	O2G-C2G	-2.01	1.41	1.46
26	D	407	SQD	O6-C1	2.01	1.43	1.40
23	B	605	CLA	C4D-CHA	2.01	1.47	1.38
23	b	608	CLA	C4A-NA	-2.01	1.34	1.38
23	C	502	CLA	CAA-C2A	2.01	1.57	1.54
23	c	909	CLA	C4D-CHA	2.01	1.47	1.38
23	b	614	CLA	C1A-NA	-2.01	1.27	1.32
23	c	913	CLA	C1D-C2D	2.01	1.47	1.42
23	B	606	CLA	CHD-C4C	2.01	1.45	1.41
23	A	410	CLA	C4D-CHA	2.01	1.47	1.38
28	d	405	PL9	C2-C3	2.00	1.40	1.34
30	F	102	LMT	O1'-C1'	2.01	1.43	1.40
23	d	403	CLA	C4D-CHA	2.00	1.47	1.38
25	t	101	BCR	C12-C13	2.00	1.50	1.45
23	A	406	CLA	CMC-C2C	2.00	1.55	1.50
34	c	919	DGD	O2D-C2D	2.00	1.47	1.43

All (3094) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	907	CLA	CHD-C4C-NC	11.31	132.18	124.28
26	a	416	SQD	O9-S-C6	11.12	116.66	106.83
23	C	502	CLA	CHD-C4C-NC	11.12	132.05	124.28
23	C	510	CLA	CHD-C4C-NC	10.52	131.63	124.28
23	B	609	CLA	C2B-C1B-NB	10.43	116.46	109.50
23	B	608	CLA	C2B-C1B-NB	10.20	116.31	109.50
26	a	416	SQD	O6-C1-C2	10.19	121.21	108.15
23	C	501	CLA	O2D-CGD-O1D	-10.19	103.33	123.79
23	B	604	CLA	CHD-C4C-NC	10.09	131.33	124.28
23	c	903	CLA	C2B-C1B-NB	10.02	116.19	109.50
23	B	604	CLA	C2B-C1B-NB	9.96	116.15	109.50
23	d	403	CLA	C2B-C1B-NB	9.93	116.14	109.50
23	d	402	CLA	C2B-C1B-NB	9.84	116.07	109.50
26	D	407	SQD	O6-C1-C2	9.81	120.72	108.15
23	b	613	CLA	C2B-C1B-NB	9.80	116.04	109.50
23	A	407	CLA	C2B-C1B-NB	9.76	116.02	109.50
23	B	611	CLA	C2B-C1B-NB	9.72	115.99	109.50
23	A	410	CLA	CHD-C4C-NC	9.71	131.07	124.28
33	B	631	HTG	C1'-S1-C1	9.71	114.28	100.19
23	c	910	CLA	C2B-C1B-NB	9.67	115.96	109.50
23	B	602	CLA	C2B-C1B-NB	9.64	115.94	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	522	HTG	C1'-S1-C1	9.53	114.03	100.19
23	b	606	CLA	C2B-C1B-NB	9.50	115.84	109.50
23	b	618	CLA	C2B-C1B-NB	9.42	115.79	109.50
23	A	405	CLA	C2B-C1B-NB	9.37	115.75	109.50
23	A	410	CLA	C2B-C1B-NB	9.25	115.68	109.50
23	c	907	CLA	C2B-C1B-NB	9.16	115.62	109.50
33	B	626	HTG	C1'-S1-C1	9.08	113.37	100.19
23	B	612	CLA	C2B-C1B-NB	9.06	115.55	109.50
23	B	604	CLA	C2C-C1C-NC	9.06	117.54	110.22
23	A	406	CLA	C2C-C1C-NC	9.05	117.53	110.22
24	A	408	PHO	C3D-C2D-C1D	-9.01	96.27	106.91
23	B	602	CLA	CHD-C4C-NC	8.86	130.47	124.28
23	B	615	CLA	C2B-C1B-NB	8.84	115.40	109.50
23	B	605	CLA	C2C-C1C-NC	8.83	117.35	110.22
26	B	621	SQD	O6-C1-C2	8.78	119.41	108.15
23	a	414	CLA	C2C-C1C-NC	8.73	117.27	110.22
26	L	103	SQD	O7-S-C6	8.64	114.47	106.83
23	c	912	CLA	CHD-C4C-NC	8.64	130.32	124.28
23	B	607	CLA	CHD-C4C-NC	8.64	130.32	124.28
23	B	612	CLA	CHD-C4C-NC	8.62	130.31	124.28
23	b	619	CLA	C2B-C1B-NB	8.61	115.25	109.50
23	c	902	CLA	C2B-C1B-NB	8.59	115.24	109.50
26	A	412	SQD	O6-C1-C2	8.59	119.16	108.15
23	c	905	CLA	C2B-C1B-NB	8.57	115.22	109.50
23	b	604	CLA	C2B-C1B-NB	8.51	115.18	109.50
23	B	609	CLA	C2C-C1C-NC	8.48	117.07	110.22
33	c	924	HTG	C1'-S1-C1	8.46	112.47	100.19
23	B	606	CLA	C2B-C1B-NB	8.45	115.14	109.50
23	D	402	CLA	CHD-C4C-NC	8.45	130.18	124.28
23	C	511	CLA	C2B-C1B-NB	8.39	115.11	109.50
23	C	510	CLA	C2B-C1B-NB	8.39	115.11	109.50
23	c	909	CLA	C2B-C1B-NB	8.37	115.09	109.50
23	B	614	CLA	C1D-C2D-C3D	-8.32	98.82	106.97
23	a	410	CLA	CHD-C4C-NC	8.31	130.09	124.28
23	b	606	CLA	CHD-C4C-NC	8.24	130.04	124.28
23	d	402	CLA	C2C-C1C-NC	8.23	116.87	110.22
33	b	627	HTG	C1'-S1-C1	8.19	112.07	100.19
24	A	409	PHO	C3D-C2D-C1D	-8.12	97.32	106.91
33	c	923	HTG	C1'-S1-C1	8.11	111.96	100.19
23	a	411	CLA	C2C-C1C-NC	8.07	116.73	110.22
23	a	409	CLA	C1D-C2D-C3D	-8.03	99.10	106.97
23	b	608	CLA	C2C-C1C-NC	8.03	116.71	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CHD-C4C-NC	8.00	129.87	124.28
26	A	412	SQD	O9-S-C6	7.99	113.89	106.83
23	b	606	CLA	C2C-C1C-NC	7.98	116.67	110.22
23	C	502	CLA	C2B-C1B-NB	7.98	114.83	109.50
23	D	403	CLA	C2B-C1B-NB	7.96	114.81	109.50
23	d	403	CLA	CHD-C4C-NC	7.93	129.82	124.28
23	C	509	CLA	C2B-C1B-NB	7.92	114.79	109.50
23	C	504	CLA	C2C-C1C-NC	7.86	116.57	110.22
23	b	619	CLA	CHD-C4C-NC	7.85	129.76	124.28
23	c	908	CLA	CHD-C4C-NC	7.84	129.76	124.28
23	c	903	CLA	CHD-C4C-NC	7.83	129.75	124.28
23	D	402	CLA	C1D-C2D-C3D	-7.81	99.32	106.97
33	u	201	HTG	C1'-S1-C1	7.80	111.51	100.19
23	c	909	CLA	C1D-C2D-C3D	-7.79	99.33	106.97
23	b	609	CLA	C2B-C1B-NB	7.78	114.70	109.50
23	b	616	CLA	C1D-C2D-C3D	-7.76	99.37	106.97
23	C	509	CLA	C2C-C1C-NC	7.75	116.48	110.22
23	c	902	CLA	CHD-C4C-NC	7.73	129.68	124.28
23	a	411	CLA	C1D-C2D-C3D	-7.71	99.42	106.97
23	B	615	CLA	CHD-C4C-NC	7.67	129.64	124.28
23	a	414	CLA	C2B-C1B-NB	7.65	114.61	109.50
23	C	503	CLA	C2B-C1B-NB	7.64	114.60	109.50
23	B	617	CLA	C2B-C1B-NB	7.63	114.59	109.50
23	c	904	CLA	C1D-C2D-C3D	-7.60	99.52	106.97
23	C	507	CLA	C2B-C1B-NB	7.59	114.57	109.50
26	B	621	SQD	O7-S-C6	7.57	113.52	106.83
23	B	616	CLA	C2B-C1B-NB	7.57	114.56	109.50
23	b	604	CLA	CHD-C4C-NC	7.53	129.54	124.28
23	B	614	CLA	CHD-C4C-NC	7.51	129.53	124.28
23	B	612	CLA	C2C-C1C-NC	7.50	116.28	110.22
23	c	913	CLA	C2B-C1B-NB	7.47	114.49	109.50
23	C	505	CLA	C2C-C1C-NC	7.47	116.25	110.22
24	A	409	PHO	C3D-C4D-ND	7.44	116.19	106.81
23	C	501	CLA	O2D-CGD-CBD	7.44	126.37	111.34
23	b	614	CLA	C2B-C1B-NB	7.41	114.45	109.50
23	b	616	CLA	C2B-C1B-NB	7.40	114.44	109.50
37	F	101	HEM	CBD-CAD-C3D	-7.39	98.46	114.51
23	B	611	CLA	CHD-C4C-NC	7.39	129.45	124.28
23	C	511	CLA	C1D-C2D-C3D	-7.38	99.74	106.97
23	c	914	CLA	C2B-C1B-NB	7.38	114.43	109.50
26	A	418	SQD	O9-S-C6	7.38	113.35	106.83
23	b	610	CLA	C1D-C2D-C3D	-7.37	99.75	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C1D-C2D-C3D	-7.32	99.80	106.97
23	A	406	CLA	C1D-C2D-C3D	-7.30	99.82	106.97
23	a	410	CLA	C2B-C1B-NB	7.27	114.36	109.50
23	b	607	CLA	C2C-C1C-NC	7.25	116.08	110.22
23	B	606	CLA	C2C-C1C-NC	7.25	116.07	110.22
23	b	615	CLA	CAC-C3C-C4C	7.24	135.72	124.85
23	C	506	CLA	C2C-C1C-NC	7.24	116.07	110.22
24	A	408	PHO	C3D-C4D-ND	7.24	115.93	106.81
23	b	605	CLA	C2B-C1B-NB	7.21	114.32	109.50
23	B	608	CLA	C1D-C2D-C3D	-7.21	99.90	106.97
24	a	413	PHO	C3D-C2D-C1D	-7.20	98.40	106.91
23	b	611	CLA	C2B-C1B-NB	7.20	114.31	109.50
23	C	501	CLA	C1D-C2D-C3D	-7.18	99.93	106.97
23	B	617	CLA	C1D-C2D-C3D	-7.18	99.93	106.97
23	A	410	CLA	C2C-C1C-NC	7.17	116.01	110.22
23	c	906	CLA	C2B-C1B-NB	7.13	114.26	109.50
23	B	616	CLA	C1D-C2D-C3D	-7.13	99.99	106.97
23	c	905	CLA	C1D-C2D-C3D	-7.12	99.99	106.97
23	C	507	CLA	CHD-C4C-NC	7.09	129.24	124.28
23	C	512	CLA	C1D-C2D-C3D	-7.09	100.02	106.97
23	c	912	CLA	C2B-C1B-NB	7.06	114.21	109.50
23	b	616	CLA	C2C-C1C-NC	7.03	115.90	110.22
23	B	603	CLA	CHD-C4C-NC	7.02	129.19	124.28
24	a	413	PHO	C3D-C4D-ND	7.02	115.67	106.81
23	c	907	CLA	C1D-C2D-C3D	-7.02	100.09	106.97
24	a	412	PHO	C3D-C2D-C1D	-7.01	98.63	106.91
33	C	521	HTG	C1'-S1-C1	7.01	110.37	100.19
23	b	608	CLA	C1D-C2D-C3D	-6.99	100.12	106.97
23	C	513	CLA	C2B-C1B-NB	6.98	114.16	109.50
23	B	607	CLA	C1D-C2D-C3D	-6.96	100.15	106.97
23	a	410	CLA	C1D-C2D-C3D	-6.95	100.16	106.97
23	a	414	CLA	CHD-C4C-NC	6.95	129.13	124.28
23	b	617	CLA	C2B-C1B-NB	6.94	114.13	109.50
23	B	613	CLA	C1D-C2D-C3D	-6.94	100.17	106.97
23	c	906	CLA	CHD-C4C-NC	6.93	129.13	124.28
23	c	907	CLA	CHD-C4C-C3C	-6.92	114.33	124.97
23	b	619	CLA	C1D-C2D-C3D	-6.92	100.19	106.97
33	d	401	HTG	C1'-S1-C1	6.91	110.23	100.19
23	C	506	CLA	CHD-C4C-NC	6.91	129.11	124.28
23	A	407	CLA	C1D-C2D-C3D	-6.90	100.21	106.97
23	b	613	CLA	C1D-C2D-C3D	-6.83	100.28	106.97
23	B	612	CLA	C1D-C2D-C3D	-6.83	100.28	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	103	SQD	O6-C1-C2	6.81	116.88	108.15
23	C	501	CLA	C2B-C1B-NB	6.81	114.05	109.50
23	D	402	CLA	C4B-CHC-C1C	-6.79	118.54	127.47
23	B	602	CLA	C1D-C2D-C3D	-6.79	100.32	106.97
24	A	409	PHO	C1B-C2B-C3B	-6.78	100.28	107.10
26	L	103	SQD	O9-S-C6	6.77	112.81	106.83
23	b	606	CLA	C1D-C2D-C3D	-6.76	100.35	106.97
23	C	503	CLA	C1D-C2D-C3D	-6.75	100.35	106.97
23	c	908	CLA	C1D-C2D-C3D	-6.74	100.36	106.97
23	b	609	CLA	C1D-C2D-C3D	-6.74	100.37	106.97
23	b	605	CLA	C1D-C2D-C3D	-6.73	100.38	106.97
23	b	617	CLA	C1D-C2D-C3D	-6.72	100.38	106.97
23	b	607	CLA	C2B-C1B-NB	6.72	113.99	109.50
23	B	614	CLA	C2B-C1B-NB	6.71	113.98	109.50
23	B	616	CLA	C2C-C1C-NC	6.70	115.63	110.22
37	f	101	HEM	CBA-CAA-C2A	-6.70	101.48	112.63
23	C	506	CLA	C1D-C2D-C3D	-6.70	100.41	106.97
23	c	913	CLA	C1D-C2D-C3D	-6.67	100.44	106.97
23	B	607	CLA	C2C-C1C-NC	6.67	115.60	110.22
23	b	618	CLA	C1D-C2D-C3D	-6.65	100.45	106.97
23	b	611	CLA	C1D-C2D-C3D	-6.65	100.46	106.97
23	b	619	CLA	CHD-C4C-C3C	-6.63	114.78	124.97
23	A	407	CLA	C2C-C1C-NC	6.63	115.57	110.22
23	C	502	CLA	CHD-C4C-C3C	-6.60	114.83	124.97
23	C	501	CLA	C2C-C1C-NC	6.60	115.55	110.22
23	b	609	CLA	CHD-C4C-NC	6.60	128.89	124.28
23	c	903	CLA	C2D-C1D-ND	6.59	117.08	109.56
33	V	202	HTG	O5-C1-C2	-6.59	101.94	110.42
23	b	617	CLA	CHD-C4C-NC	6.55	128.86	124.28
23	a	409	CLA	CHD-C4C-NC	6.55	128.86	124.28
23	b	615	CLA	C1D-C2D-C3D	-6.54	100.57	106.97
23	C	505	CLA	CHD-C4C-NC	6.51	128.83	124.28
23	a	410	CLA	C2C-C1C-NC	6.49	115.46	110.22
23	b	617	CLA	C2D-C1D-ND	6.49	116.96	109.56
33	B	630	HTG	C1'-S1-C1	6.48	109.60	100.19
23	B	603	CLA	C1D-C2D-C3D	-6.47	100.64	106.97
23	D	402	CLA	C2C-C1C-NC	6.46	115.44	110.22
23	B	617	CLA	C2C-C1C-NC	6.46	115.44	110.22
23	B	607	CLA	C2B-C1B-NB	6.44	113.80	109.50
23	b	612	CLA	C2C-C1C-NC	6.42	115.40	110.22
23	b	618	CLA	CHD-C4C-NC	6.41	128.76	124.28
23	B	604	CLA	CHD-C4C-C3C	-6.40	115.14	124.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	C2B-C1B-NB	6.40	113.77	109.50
23	d	403	CLA	C1D-C2D-C3D	-6.39	100.71	106.97
23	B	611	CLA	C1D-C2D-C3D	-6.39	100.71	106.97
23	C	504	CLA	C1D-C2D-C3D	-6.38	100.72	106.97
23	c	914	CLA	CHD-C4C-NC	6.38	128.74	124.28
23	c	904	CLA	C2B-C1B-NB	6.38	113.76	109.50
23	B	607	CLA	C4B-CHC-C1C	-6.38	119.08	127.47
23	C	502	CLA	C1D-C2D-C3D	-6.36	100.74	106.97
23	B	610	CLA	C2B-C1B-NB	6.36	113.75	109.50
23	A	410	CLA	CBD-CHA-C1A	6.35	137.07	128.77
23	B	610	CLA	C2C-C1C-NC	6.35	115.35	110.22
23	b	618	CLA	C2C-C1C-NC	6.35	115.35	110.22
23	d	402	CLA	C4B-CHC-C1C	-6.34	119.12	127.47
23	C	513	CLA	C1D-C2D-C3D	-6.34	100.76	106.97
23	b	610	CLA	CHD-C4C-NC	6.33	128.71	124.28
23	B	606	CLA	C1D-C2D-C3D	-6.33	100.77	106.97
23	A	406	CLA	C2B-C1B-NB	6.32	113.72	109.50
23	d	402	CLA	C1D-C2D-C3D	-6.32	100.78	106.97
34	D	406	DGD	O2G-C1B-C2B	6.30	124.96	111.54
23	A	410	CLA	C1D-C2D-C3D	-6.30	100.80	106.97
23	c	902	CLA	C1D-C2D-C3D	-6.29	100.81	106.97
26	a	401	SQD	O6-C1-C2	6.28	116.20	108.15
23	c	908	CLA	C2B-C1B-NB	6.27	113.69	109.50
23	c	905	CLA	C2D-C1D-ND	6.26	116.70	109.56
23	c	903	CLA	C1D-C2D-C3D	-6.25	100.85	106.97
23	c	906	CLA	C1D-C2D-C3D	-6.24	100.86	106.97
23	B	612	CLA	CHD-C4C-C3C	-6.23	115.40	124.97
23	c	910	CLA	CBD-CHA-C1A	6.23	136.91	128.77
23	A	405	CLA	C1D-C2D-C3D	-6.23	100.87	106.97
23	b	613	CLA	C2D-C1D-ND	6.21	116.64	109.56
23	b	611	CLA	C2C-C1C-NC	6.19	115.22	110.22
23	C	503	CLA	CHD-C4C-NC	6.19	128.61	124.28
23	c	911	CLA	C1D-C2D-C3D	-6.19	100.91	106.97
26	A	412	SQD	O7-S-C6	-6.17	101.37	106.83
23	B	609	CLA	C1D-C2D-C3D	-6.15	100.94	106.97
23	a	411	CLA	C2B-C1B-NB	6.15	113.60	109.50
23	c	908	CLA	C2C-C1C-NC	6.15	115.18	110.22
26	A	412	SQD	C1-C2-C3	-6.14	98.09	109.99
33	V	202	HTG	O5-C1-S1	6.14	119.56	108.52
23	C	507	CLA	C1D-C2D-C3D	-6.13	100.96	106.97
23	B	611	CLA	C2C-C1C-NC	6.12	115.16	110.22
23	b	617	CLA	CBD-CHA-C1A	6.11	136.75	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	912	CLA	C2C-C1C-NC	6.10	115.15	110.22
23	C	510	CLA	CHD-C4C-C3C	-6.10	115.60	124.97
23	b	613	CLA	CHD-C4C-NC	6.09	128.53	124.28
23	d	402	CLA	C3B-C4B-CHC	-6.08	114.48	126.00
23	C	512	CLA	CHD-C4C-NC	6.08	128.53	124.28
23	C	506	CLA	CHD-C4C-C3C	-6.07	115.64	124.97
23	d	402	CLA	CHD-C4C-NC	6.07	128.52	124.28
23	c	902	CLA	C2C-C1C-NC	6.06	115.11	110.22
23	B	605	CLA	C1D-C2D-C3D	-6.06	101.04	106.97
23	b	610	CLA	C2B-C1B-NB	6.05	113.54	109.50
23	C	510	CLA	C1D-C2D-C3D	-6.05	101.05	106.97
23	B	608	CLA	CHD-C4C-NC	6.04	128.50	124.28
23	C	509	CLA	CBD-CHA-C1A	6.03	136.65	128.77
23	B	608	CLA	C4B-C3B-C2B	-6.03	100.84	107.04
23	B	610	CLA	C1D-C2D-C3D	-6.03	101.07	106.97
23	b	614	CLA	C1D-C2D-C3D	-6.02	101.07	106.97
38	H	101	RRX	C24-C23-C22	-6.02	117.21	126.22
23	B	608	CLA	C2C-C1C-NC	6.01	115.07	110.22
23	b	612	CLA	C2B-C1B-NB	6.00	113.51	109.50
23	b	613	CLA	C2C-C1C-NC	6.00	115.07	110.22
26	D	407	SQD	O9-S-C6	6.00	112.13	106.83
24	a	413	PHO	C4D-CHA-C1A	-6.00	122.43	129.57
23	C	512	CLA	C2B-C1B-NB	5.99	113.50	109.50
28	d	405	PL9	C40-C39-C41	5.98	124.48	115.39
23	b	608	CLA	CAC-C3C-C4C	5.98	133.82	124.85
23	a	409	CLA	CAC-C3C-C4C	5.96	133.80	124.85
23	B	617	CLA	CHD-C4C-NC	5.96	128.44	124.28
23	C	510	CLA	C2C-C1C-NC	5.96	115.03	110.22
23	A	410	CLA	C4B-CHC-C1C	-5.94	119.65	127.47
23	C	503	CLA	C2C-C1C-NC	5.91	115.00	110.22
23	B	615	CLA	C1D-C2D-C3D	-5.91	101.18	106.97
23	A	410	CLA	C4-C3-C5	5.90	124.35	115.39
23	b	608	CLA	C2B-C1B-NB	5.89	113.43	109.50
37	f	101	HEM	CBD-CAD-C3D	-5.88	101.75	114.51
23	B	607	CLA	CHD-C4C-C3C	-5.87	115.96	124.97
23	b	615	CLA	CHD-C4C-C3C	-5.86	115.97	124.97
23	c	902	CLA	CBD-CHA-C1A	5.83	136.39	128.77
23	c	911	CLA	C2B-C1B-NB	5.82	113.39	109.50
23	a	414	CLA	CHD-C4C-C3C	-5.82	116.03	124.97
23	c	909	CLA	C2D-C1D-ND	5.82	116.20	109.56
23	b	609	CLA	CBD-CHA-C1A	5.82	136.38	128.77
23	B	614	CLA	CBD-CHA-C1A	5.82	136.38	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	CBD-CHA-C1A	5.81	136.37	128.77
23	D	403	CLA	C1D-C2D-C3D	-5.80	101.29	106.97
28	D	405	PL9	C40-C39-C41	5.80	124.19	115.39
23	a	414	CLA	C3B-C4B-CHC	-5.79	115.03	126.00
23	B	611	CLA	CBD-CHA-C1A	5.78	136.33	128.77
37	V	201	HEM	CBD-CAD-C3D	-5.78	101.97	114.51
23	C	502	CLA	C2C-C1C-NC	5.76	114.88	110.22
23	B	617	CLA	C2D-C1D-ND	5.77	116.14	109.56
23	c	908	CLA	CHD-C4C-C3C	-5.75	116.14	124.97
23	b	617	CLA	C4B-CHC-C1C	-5.73	119.93	127.47
26	B	621	SQD	C1-O5-C5	-5.72	102.66	113.73
24	A	409	PHO	C4D-CHA-C1A	-5.72	122.75	129.57
26	a	416	SQD	C1-C2-C3	-5.71	98.93	109.99
23	C	505	CLA	C1D-C2D-C3D	-5.70	101.39	106.97
23	c	910	CLA	C2C-C1C-NC	5.69	114.82	110.22
23	B	602	CLA	CHD-C4C-C3C	-5.68	116.25	124.97
23	b	615	CLA	C2C-C1C-NC	5.68	114.81	110.22
27	A	413	LMG	O1-C1-C2	5.67	115.42	108.15
23	a	410	CLA	CHD-C4C-C3C	-5.66	116.27	124.97
23	a	409	CLA	C2C-C1C-NC	5.66	114.79	110.22
23	B	607	CLA	C2D-C1D-ND	5.65	116.00	109.56
23	c	910	CLA	C3B-C4B-CHC	-5.64	115.31	126.00
23	b	605	CLA	CHD-C4C-NC	5.63	128.22	124.28
26	a	416	SQD	C1-O5-C5	-5.63	102.85	113.73
25	C	515	BCR	C7-C8-C9	-5.62	117.81	126.22
23	a	409	CLA	C2D-C1D-ND	5.61	115.95	109.56
23	C	507	CLA	CBD-CHA-C1A	5.60	136.09	128.77
23	a	411	CLA	CBD-CHA-C1A	5.60	136.09	128.77
27	a	418	LMG	O7-C10-C11	5.59	123.45	111.54
23	C	501	CLA	CHD-C4C-NC	5.59	128.19	124.28
23	B	617	CLA	CHD-C4C-C3C	-5.58	116.39	124.97
23	D	402	CLA	C2B-C1B-CHB	-5.57	115.44	126.00
26	A	412	SQD	O8-S-C6	5.57	112.52	105.89
24	A	408	PHO	C3C-C4C-NC	5.57	118.46	109.87
23	b	614	CLA	CHD-C4C-NC	5.57	128.18	124.28
34	d	406	DGD	C3D-C4D-C5D	5.57	116.43	109.29
23	c	907	CLA	CBD-CHA-C1A	5.56	136.03	128.77
23	C	511	CLA	C2C-C1C-NC	5.54	114.70	110.22
23	d	403	CLA	CBD-CHA-C1A	5.54	136.01	128.77
23	b	615	CLA	CBD-CHA-C1A	5.54	136.01	128.77
24	A	408	PHO	C1B-C2B-C3B	-5.52	101.55	107.10
23	b	615	CLA	C3C-C4C-NC	5.52	116.80	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	412	SQD	O47-C7-C8	5.51	123.28	111.54
23	B	615	CLA	C2C-C1C-NC	5.51	114.67	110.22
23	C	508	CLA	C2B-C1B-NB	5.51	113.18	109.50
23	b	613	CLA	CBD-CHA-C1A	5.51	135.97	128.77
37	v	201	HEM	CBD-CAD-C3D	-5.51	102.56	114.51
23	c	902	CLA	C2D-C1D-ND	5.51	115.84	109.56
23	C	506	CLA	CBD-CHA-C1A	5.49	135.94	128.77
26	A	412	SQD	C1-O5-C5	-5.49	103.12	113.73
23	B	613	CLA	C2C-C1C-NC	5.49	114.65	110.22
23	b	606	CLA	CHD-C4C-C3C	-5.48	116.55	124.97
23	B	605	CLA	CBD-CHA-C1A	5.48	135.93	128.77
23	c	913	CLA	CHD-C4C-NC	5.48	128.11	124.28
23	c	908	CLA	O2D-CGD-CBD	5.47	122.39	111.34
26	a	401	SQD	C1-O5-C5	-5.47	103.15	113.73
25	D	404	BCR	C7-C8-C9	-5.47	118.03	126.22
26	B	621	SQD	O9-S-C6	5.47	111.66	106.83
23	b	606	CLA	C4-C3-C5	5.47	123.69	115.39
23	b	617	CLA	O2D-CGD-CBD	5.47	122.38	111.34
33	B	625	HTG	C1'-S1-C1	5.46	108.12	100.19
23	B	609	CLA	C2D-C1D-ND	5.46	115.79	109.56
23	b	614	CLA	C2C-C1C-NC	5.46	114.63	110.22
23	B	604	CLA	C1D-C2D-C3D	-5.46	101.62	106.97
23	B	614	CLA	C2C-C1C-NC	5.46	114.63	110.22
23	b	616	CLA	CHD-C4C-NC	5.45	128.09	124.28
33	V	202	HTG	C1-O5-C5	-5.43	102.03	112.78
23	b	604	CLA	C1D-C2D-C3D	-5.42	101.66	106.97
23	d	403	CLA	C2C-C1C-NC	5.41	114.59	110.22
23	b	619	CLA	O2D-CGD-CBD	5.41	122.28	111.34
24	a	413	PHO	C1B-C2B-C3B	-5.41	101.66	107.10
23	c	905	CLA	C2C-C1C-NC	5.40	114.58	110.22
23	C	505	CLA	C2B-C1B-NB	5.39	113.10	109.50
23	A	410	CLA	C2D-C1D-ND	5.39	115.71	109.56
23	C	507	CLA	C3B-C2B-C1B	-5.39	100.72	106.69
23	A	407	CLA	C2B-C3B-CAB	5.38	138.33	127.33
23	a	414	CLA	C1D-C2D-C3D	-5.36	101.71	106.97
23	A	405	CLA	C2D-C1D-ND	5.36	115.68	109.56
23	b	615	CLA	C4B-CHC-C1C	-5.36	120.42	127.47
23	C	504	CLA	C2B-C1B-NB	5.36	113.08	109.50
23	B	609	CLA	C4B-NB-C1B	-5.36	101.96	107.12
30	C	520	LMT	O1B-C4'-C3'	5.35	120.73	107.17
23	c	903	CLA	CHD-C4C-C3C	-5.35	116.76	124.97
23	b	618	CLA	CMD-C2D-C3D	5.34	135.22	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	CHD-C4C-C3C	-5.34	116.77	124.97
23	B	602	CLA	O2D-CGD-CBD	5.33	122.12	111.34
33	V	202	HTG	C1-C2-C3	-5.33	99.60	110.72
23	b	608	CLA	C4-C3-C5	5.33	123.49	115.39
23	C	502	CLA	C4B-CHC-C1C	-5.33	120.46	127.47
23	c	909	CLA	CBD-CHA-C1A	5.33	135.74	128.77
33	D	414	HTG	C1'-S1-C1	5.32	107.92	100.19
23	c	906	CLA	C3B-C2B-C1B	-5.32	100.79	106.69
24	A	409	PHO	C4C-C3C-C2C	-5.31	100.67	106.83
26	a	416	SQD	O47-C7-C8	5.31	122.85	111.54
23	b	618	CLA	C3B-C4B-CHC	-5.31	115.94	126.00
23	A	405	CLA	CMD-C2D-C3D	5.30	135.16	125.16
24	a	412	PHO	C1B-C2B-C3B	-5.29	101.78	107.10
23	c	910	CLA	C1D-C2D-C3D	-5.28	101.80	106.97
27	B	622	LMG	O7-C10-C11	5.28	122.79	111.54
24	A	408	PHO	C2D-C1D-ND	5.27	118.60	107.96
23	B	607	CLA	CBD-CHA-C1A	5.27	135.66	128.77
33	c	924	HTG	C1-O5-C5	5.25	123.17	112.78
23	a	411	CLA	CAC-C3C-C4C	5.25	132.73	124.85
23	B	602	CLA	C2C-C1C-NC	5.25	114.46	110.22
23	B	611	CLA	C2D-C1D-ND	5.24	115.54	109.56
23	A	407	CLA	CAC-C3C-C4C	5.23	132.71	124.85
23	c	914	CLA	C1D-C2D-C3D	-5.23	101.84	106.97
25	B	620	BCR	C38-C26-C25	-5.21	118.61	124.50
33	B	624	HTG	C2-C1-S1	5.21	116.84	110.97
33	O	303	HTG	C1'-S1-C1	5.21	107.75	100.19
23	c	907	CLA	C2D-C1D-ND	5.19	115.48	109.56
23	c	906	CLA	C2C-C1C-NC	5.18	114.41	110.22
23	D	402	CLA	CHD-C4C-C3C	-5.18	117.01	124.97
33	C	522	HTG	C1-O5-C5	5.17	123.00	112.78
23	B	602	CLA	CBD-CHA-C1A	5.17	135.52	128.77
23	C	504	CLA	CHD-C4C-NC	5.17	127.89	124.28
24	A	408	PHO	C4C-C3C-C2C	-5.16	100.84	106.83
23	b	616	CLA	CBD-CHA-C1A	5.16	135.52	128.77
23	c	912	CLA	C1D-C2D-C3D	-5.16	101.91	106.97
23	d	402	CLA	CHD-C4C-C3C	-5.16	117.05	124.97
23	B	604	CLA	C1C-C2C-C3C	-5.15	100.48	106.96
26	A	418	SQD	O6-C1-C2	5.14	114.74	108.15
23	b	604	CLA	O2D-CGD-CBD	5.13	121.71	111.34
23	c	912	CLA	CBD-CHA-C1A	5.13	135.48	128.77
23	c	910	CLA	CHD-C4C-NC	5.13	127.87	124.28
23	D	403	CLA	C2C-C1C-NC	5.13	114.36	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402	CLA	CHB-C1B-NB	5.12	133.40	124.70
23	B	615	CLA	CAC-C3C-C4C	5.12	132.54	124.85
36	D	408	LHG	O8-C23-O10	-5.11	110.13	123.48
23	B	610	CLA	CHD-C4C-NC	5.10	127.84	124.28
23	d	402	CLA	C4-C3-C5	5.10	123.13	115.39
23	c	904	CLA	C2C-C1C-NC	5.09	114.33	110.22
23	B	606	CLA	C2D-C1D-ND	5.09	115.37	109.56
23	b	605	CLA	CMB-C2B-C3B	5.09	134.75	125.16
23	b	610	CLA	C2C-C1C-NC	5.09	114.33	110.22
23	a	409	CLA	C3B-C2B-C1B	-5.09	101.05	106.69
27	C	519	LMG	O1-C7-C8	-5.08	98.89	110.99
23	b	617	CLA	C2C-C1C-NC	5.08	114.32	110.22
23	C	507	CLA	C2C-C1C-NC	5.08	114.32	110.22
23	C	512	CLA	CBD-CHA-C1A	5.07	135.40	128.77
30	a	402	LMT	C1'-O5'-C5'	5.06	123.53	113.73
23	B	614	CLA	C2D-C1D-ND	5.06	115.33	109.56
23	c	908	CLA	O2D-CGD-O1D	-5.06	113.64	123.79
23	a	414	CLA	C4B-CHC-C1C	-5.05	120.82	127.47
23	b	604	CLA	C2C-C1C-NC	5.04	114.30	110.22
23	c	912	CLA	CHD-C4C-C3C	-5.04	117.23	124.97
23	c	903	CLA	C3B-C2B-C1B	-5.04	101.10	106.69
23	B	613	CLA	CAC-C3C-C4C	5.04	132.41	124.85
23	D	403	CLA	C2D-C1D-ND	5.03	115.29	109.56
23	D	402	CLA	CMD-C2D-C3D	5.03	134.63	125.16
23	B	609	CLA	CBD-CHA-C1A	5.02	135.34	128.77
23	C	506	CLA	O2D-CGD-CBD	5.02	121.49	111.34
23	C	511	CLA	CHD-C4C-NC	5.02	127.79	124.28
23	d	402	CLA	CBD-CHA-C1A	5.02	135.33	128.77
23	B	605	CLA	C1C-C2C-C3C	-5.02	100.65	106.96
23	b	611	CLA	CHD-C4C-NC	5.02	127.79	124.28
23	b	616	CLA	C1-C2-C3	-5.01	117.54	126.23
23	C	508	CLA	CBD-CHA-C1A	5.00	135.31	128.77
23	c	913	CLA	CBD-CHA-C1A	5.00	135.31	128.77
23	b	605	CLA	CMD-C2D-C3D	5.00	134.59	125.16
23	b	606	CLA	C3B-C4B-CHC	-4.99	116.53	126.00
23	B	609	CLA	C4B-CHC-C1C	-4.99	120.91	127.47
23	C	501	CLA	CBD-CHA-C1A	4.99	135.29	128.77
23	a	414	CLA	CAC-C3C-C4C	4.98	132.33	124.85
23	c	903	CLA	C2C-C1C-NC	4.98	114.24	110.22
23	A	406	CLA	C2A-C1A-NA	4.98	117.70	111.33
23	C	513	CLA	CHD-C4C-NC	4.97	127.76	124.28
23	b	605	CLA	C2C-C1C-NC	4.97	114.23	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	CAC-C3C-C4C	4.96	132.30	124.85
23	B	613	CLA	C4B-CHC-C1C	-4.96	120.95	127.47
23	B	617	CLA	C3B-C2B-C1B	-4.96	101.19	106.69
23	B	616	CLA	CHD-C4C-NC	4.95	127.74	124.28
23	d	403	CLA	C3B-C2B-C1B	-4.94	101.21	106.69
23	A	410	CLA	C3B-C4B-CHC	-4.94	116.63	126.00
23	c	911	CLA	C2D-C1D-ND	4.94	115.20	109.56
23	B	613	CLA	C2B-C1B-NB	4.94	112.80	109.50
23	C	509	CLA	C3B-C2B-C1B	-4.94	101.21	106.69
23	A	406	CLA	C1C-C2C-C3C	-4.94	100.75	106.96
23	C	508	CLA	CHD-C4C-NC	4.94	127.73	124.28
23	C	511	CLA	CBD-CHA-C1A	4.94	135.22	128.77
33	b	602	HTG	C1'-S1-C1	4.93	107.34	100.19
23	B	612	CLA	C4B-CHC-C1C	-4.92	121.00	127.47
23	B	610	CLA	CBD-CHA-C1A	4.92	135.20	128.77
23	C	504	CLA	C1C-C2C-C3C	-4.92	100.78	106.96
23	B	606	CLA	C3B-C2B-C1B	-4.91	101.24	106.69
28	a	419	PL9	C7-C3-C4	4.91	120.85	116.92
24	a	413	PHO	O2D-CGD-CBD	4.91	121.26	111.34
23	c	906	CLA	CHD-C4C-C3C	-4.91	117.43	124.97
23	c	907	CLA	C3B-C2B-C1B	-4.90	101.25	106.69
23	b	609	CLA	C2C-C1C-NC	4.90	114.18	110.22
23	B	609	CLA	C3B-C4B-NB	4.90	115.54	109.21
25	b	620	BCR	C33-C5-C6	-4.89	118.97	124.50
23	a	411	CLA	C4B-CHC-C1C	-4.89	121.03	127.47
24	A	409	PHO	C3C-C4C-NC	4.89	117.41	109.87
23	d	403	CLA	C2D-C1D-ND	4.89	115.14	109.56
23	b	619	CLA	C2C-C1C-NC	4.89	114.17	110.22
23	A	405	CLA	CBD-CHA-C1A	4.87	135.14	128.77
23	B	609	CLA	O2D-CGD-CBD	4.86	121.17	111.34
23	A	410	CLA	CHD-C4C-C3C	-4.86	117.51	124.97
23	b	606	CLA	O2D-CGD-O1D	-4.86	114.03	123.79
27	Z	101	LMG	O7-C10-C11	4.85	121.88	111.54
33	b	626	HTG	C2-C1-S1	4.84	116.42	110.97
23	C	511	CLA	C2D-C1D-ND	4.84	115.08	109.56
23	B	611	CLA	CHB-C4A-NA	4.84	131.13	124.38
26	D	407	SQD	O7-S-C6	4.84	111.11	106.83
24	a	412	PHO	C3D-C4D-ND	4.83	112.90	106.81
23	a	409	CLA	CBD-CHA-C1A	4.83	135.09	128.77
23	B	616	CLA	CHD-C4C-C3C	-4.83	117.55	124.97
23	b	612	CLA	C1D-C2D-C3D	-4.83	102.24	106.97
23	D	402	CLA	C1B-CHB-C4A	-4.83	120.56	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	911	CLA	CBD-CHA-C1A	4.83	135.08	128.77
23	B	602	CLA	C2D-C1D-ND	4.83	115.06	109.56
23	D	403	CLA	CHD-C4C-NC	4.82	127.65	124.28
23	C	510	CLA	CBD-CHA-C1A	4.82	135.07	128.77
23	c	905	CLA	CBD-CHA-C1A	4.82	135.07	128.77
30	m	102	LMT	O1'-C1'-C2'	4.82	114.33	108.15
23	C	505	CLA	CHD-C4C-C3C	-4.82	117.57	124.97
23	b	619	CLA	C3B-C2B-C1B	-4.82	101.35	106.69
23	a	410	CLA	C2D-C1D-ND	4.82	115.06	109.56
26	a	401	SQD	O9-S-C6	4.81	111.08	106.83
23	B	604	CLA	CBD-CHA-C1A	4.80	135.05	128.77
25	K	102	BCR	C11-C10-C9	-4.80	120.35	127.29
23	B	605	CLA	C3C-C4C-NC	4.80	115.94	110.15
23	C	509	CLA	C3B-C4B-CHC	-4.80	116.90	126.00
23	b	616	CLA	C2D-C1D-ND	4.79	115.03	109.56
23	A	406	CLA	CHD-C4C-NC	4.79	127.63	124.28
23	a	414	CLA	CBD-CHA-C1A	4.79	135.03	128.77
23	B	604	CLA	C3B-C4B-CHC	-4.79	116.92	126.00
23	B	607	CLA	C3B-C4B-CHC	-4.78	116.93	126.00
23	B	612	CLA	CMC-C2C-C1C	4.78	131.77	124.95
33	D	414	HTG	C2-C1-S1	4.78	116.35	110.97
23	c	903	CLA	C4D-ND-C1D	-4.78	100.79	106.57
23	a	411	CLA	C3C-C4C-NC	4.78	115.91	110.15
23	B	611	CLA	CHD-C4C-C3C	-4.78	117.64	124.97
23	B	604	CLA	C3B-C4B-NB	4.77	115.37	109.21
23	b	605	CLA	C2D-C1D-ND	4.76	114.98	109.56
23	c	913	CLA	O2D-CGD-CBD	4.75	120.94	111.34
23	b	608	CLA	C3C-C4C-NC	4.75	115.88	110.15
23	b	607	CLA	CBD-CHA-C1A	4.75	134.98	128.77
23	A	406	CLA	CMD-C2D-C3D	4.75	134.11	125.16
27	B	622	LMG	O8-C28-C29	4.75	126.42	111.90
23	b	608	CLA	CBD-CHA-C1A	4.74	134.97	128.77
23	B	616	CLA	C3B-C2B-C1B	-4.74	101.43	106.69
23	d	403	CLA	O2D-CGD-CBD	4.74	120.92	111.34
23	C	503	CLA	C3B-C2B-C1B	-4.74	101.44	106.69
23	B	604	CLA	CMC-C2C-C1C	4.73	131.70	124.95
23	c	904	CLA	CHD-C4C-NC	4.73	127.59	124.28
23	B	613	CLA	C2D-C1D-ND	4.73	114.96	109.56
23	b	610	CLA	CHD-C4C-C3C	-4.73	117.70	124.97
23	c	902	CLA	C3B-C2B-C1B	-4.73	101.44	106.69
24	a	412	PHO	C3C-C4C-NC	4.73	117.16	109.87
23	B	604	CLA	C4B-NB-C1B	-4.73	102.57	107.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	CHD-C4C-C3C	-4.73	117.71	124.97
23	b	615	CLA	C2B-C1B-NB	4.72	112.65	109.50
23	B	614	CLA	CHD-C4C-C3C	-4.72	117.73	124.97
23	b	618	CLA	C3B-C2B-C1B	-4.71	101.46	106.69
23	C	506	CLA	C3B-CAB-CBB	-4.71	116.19	125.95
23	B	610	CLA	O2D-CGD-O1D	-4.71	114.33	123.79
23	C	503	CLA	CHD-C4C-C3C	-4.70	117.76	124.97
23	b	608	CLA	CHD-C4C-C3C	-4.69	117.76	124.97
23	B	617	CLA	CAC-C3C-C4C	4.69	131.89	124.85
23	C	510	CLA	C3B-C4B-CHC	-4.69	117.10	126.00
23	b	608	CLA	C2A-C1A-NA	4.69	117.33	111.33
23	b	616	CLA	CAC-C3C-C4C	4.69	131.89	124.85
23	c	906	CLA	O2D-CGD-O1D	-4.69	114.38	123.79
24	a	413	PHO	O2D-CGD-O1D	-4.67	114.40	123.79
23	B	609	CLA	CHD-C4C-C3C	-4.67	117.80	124.97
25	B	620	BCR	C24-C23-C22	-4.67	119.23	126.22
23	c	905	CLA	CGD-CBD-CHA	-4.67	102.83	113.65
23	b	606	CLA	C2D-C1D-ND	4.66	114.88	109.56
23	b	617	CLA	O2D-CGD-O1D	-4.66	114.43	123.79
23	c	910	CLA	CHD-C4C-C3C	-4.66	117.81	124.97
23	B	610	CLA	C4B-CHC-C1C	-4.66	121.34	127.47
23	C	508	CLA	C1D-C2D-C3D	-4.66	102.41	106.97
23	c	911	CLA	C2C-C1C-NC	4.65	113.98	110.22
37	F	101	HEM	CBA-CAA-C2A	-4.65	104.89	112.63
24	a	412	PHO	C4D-CHA-C1A	-4.64	124.04	129.57
36	D	408	LHG	O8-C23-C24	4.63	126.08	111.90
23	c	908	CLA	CBD-CHA-C1A	4.63	134.82	128.77
23	c	914	CLA	C3B-C2B-C1B	-4.63	101.56	106.69
23	C	502	CLA	CBD-CHA-C1A	4.63	134.82	128.77
23	C	508	CLA	C2C-C1C-NC	4.62	113.95	110.22
23	B	610	CLA	CHD-C4C-C3C	-4.62	117.88	124.97
33	c	924	HTG	O5-C5-C4	4.62	118.31	109.73
30	t	102	LMT	O1'-C1'-C2'	4.61	114.06	108.15
23	c	903	CLA	O2D-CGD-CBD	4.61	120.66	111.34
30	a	402	LMT	O1'-C1'-C2'	4.60	114.05	108.15
24	a	412	PHO	O2D-CGD-O1D	-4.60	114.55	123.79
23	b	611	CLA	CBD-CHA-C1A	4.60	134.78	128.77
23	b	617	CLA	C1-C2-C3	-4.60	118.26	126.23
23	B	610	CLA	C3B-C2B-C1B	-4.60	101.59	106.69
23	A	407	CLA	C3B-C4B-CHC	-4.59	117.30	126.00
23	a	410	CLA	C3B-C4B-CHC	-4.58	117.31	126.00
24	a	413	PHO	CMD-C2D-C1D	4.58	135.48	128.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	PHO	CMD-C2D-C1D	4.58	135.47	128.49
23	c	913	CLA	C1-C2-C3	-4.58	118.29	126.23
23	b	608	CLA	C2D-C1D-ND	4.57	114.78	109.56
23	C	502	CLA	C2D-C1D-ND	4.57	114.78	109.56
23	b	609	CLA	C4B-CHC-C1C	-4.57	121.46	127.47
23	b	619	CLA	C2D-C1D-ND	4.57	114.77	109.56
37	F	101	HEM	CAD-C3D-C4D	4.57	132.04	125.60
23	C	511	CLA	C3B-C4B-CHC	-4.56	117.35	126.00
23	C	501	CLA	CHD-C4C-C3C	-4.56	117.97	124.97
23	c	902	CLA	O2D-CGD-O1D	-4.55	114.64	123.79
23	B	603	CLA	CHD-C4C-C3C	-4.55	117.98	124.97
23	c	909	CLA	CHD-C4C-NC	4.55	127.46	124.28
23	B	610	CLA	CAC-C3C-C4C	4.55	131.68	124.85
23	b	614	CLA	C4B-C3B-C2B	-4.54	102.37	107.04
23	b	606	CLA	C3B-C2B-C1B	-4.53	101.67	106.69
23	C	507	CLA	CHD-C4C-C3C	-4.53	118.02	124.97
23	b	607	CLA	C2D-C1D-ND	4.53	114.72	109.56
25	k	102	BCR	C7-C8-C9	-4.53	119.44	126.22
24	A	409	PHO	CAC-C3C-C4C	4.52	130.64	125.18
23	b	612	CLA	CAC-C3C-C4C	4.52	131.63	124.85
27	b	623	LMG	O8-C28-C29	4.51	125.71	111.90
23	c	908	CLA	C3B-C2B-C1B	-4.51	101.69	106.69
23	b	609	CLA	CHD-C4C-C3C	-4.51	118.05	124.97
23	b	605	CLA	C3B-C2B-C1B	-4.50	101.69	106.69
23	b	609	CLA	C2D-C1D-ND	4.50	114.69	109.56
23	b	608	CLA	CMC-C2C-C1C	4.50	131.37	124.95
26	D	407	SQD	C1-C2-C3	-4.50	101.28	109.99
23	c	902	CLA	C3B-C4B-CHC	-4.49	117.48	126.00
23	b	615	CLA	C2D-C1D-ND	4.49	114.68	109.56
23	b	611	CLA	CHD-C4C-C3C	-4.49	118.08	124.97
23	c	914	CLA	CBD-CHA-C1A	4.48	134.63	128.77
23	a	411	CLA	CHD-C4C-C3C	-4.48	118.10	124.97
30	M	101	LMT	O1'-C1'-C2'	4.47	113.88	108.15
23	b	607	CLA	CHD-C4C-C3C	-4.47	118.11	124.97
23	a	414	CLA	C2D-C1D-ND	4.47	114.66	109.56
23	B	608	CLA	C1-C2-C3	-4.47	118.48	126.23
23	A	407	CLA	CBD-CHA-C1A	4.46	134.60	128.77
23	c	903	CLA	CBD-CHA-C1A	4.46	134.60	128.77
23	c	914	CLA	CHD-C4C-C3C	-4.46	118.13	124.97
23	C	511	CLA	C4A-NA-C1A	4.46	112.67	106.38
23	c	913	CLA	C3B-C2B-C1B	-4.45	101.76	106.69
23	B	613	CLA	C3B-C2B-C1B	-4.45	101.76	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	PHO	C2D-C1D-ND	4.44	116.92	107.96
23	b	619	CLA	CBD-CHA-C1A	4.44	134.57	128.77
24	A	408	PHO	C4D-CHA-C1A	-4.44	124.28	129.57
23	c	913	CLA	C2C-C1C-NC	4.44	113.81	110.22
23	B	615	CLA	C2D-C1D-ND	4.44	114.62	109.56
23	C	504	CLA	C2D-C1D-ND	4.44	114.62	109.56
23	C	510	CLA	CGD-CBD-CHA	-4.43	103.37	113.65
23	B	604	CLA	C3B-C2B-C1B	-4.43	101.78	106.69
23	B	604	CLA	O2D-CGD-O1D	-4.42	114.91	123.79
23	B	617	CLA	O2D-CGD-O1D	-4.42	114.91	123.79
26	A	418	SQD	O48-C23-C24	4.42	125.43	111.90
23	B	615	CLA	CBD-CHA-C1A	4.42	134.55	128.77
23	B	610	CLA	CMD-C2D-C3D	4.42	133.49	125.16
23	d	402	CLA	O2D-CGD-O1D	-4.41	114.93	123.79
25	K	101	BCR	C37-C22-C23	4.41	125.22	118.09
23	C	512	CLA	C2C-C1C-NC	4.41	113.78	110.22
23	c	907	CLA	C3B-C4B-CHC	-4.41	117.65	126.00
23	c	902	CLA	C4B-CHC-C1C	-4.40	121.68	127.47
23	b	613	CLA	C3B-C2B-C1B	-4.40	101.81	106.69
23	B	604	CLA	O2D-CGD-CBD	4.40	120.23	111.34
23	b	619	CLA	C3C-C4C-NC	4.40	115.45	110.15
23	B	615	CLA	CHD-C4C-C3C	-4.40	118.22	124.97
23	b	618	CLA	C3B-CAB-CBB	-4.39	116.87	125.95
23	B	612	CLA	C3B-C4B-CHC	-4.38	117.69	126.00
33	V	202	HTG	C2-C1-S1	4.38	120.99	109.29
23	b	617	CLA	C3B-C4B-CHC	-4.37	117.72	126.00
23	c	902	CLA	C1C-C2C-C3C	-4.37	101.46	106.96
27	d	410	LMG	O7-C10-C11	4.37	120.85	111.54
23	A	405	CLA	CHD-C4C-NC	4.36	127.33	124.28
25	b	620	BCR	C7-C8-C9	-4.36	119.69	126.22
23	A	406	CLA	CHD-C4C-C3C	-4.35	118.30	124.97
23	C	512	CLA	CHD-C4C-C3C	-4.35	118.30	124.97
23	a	409	CLA	CHD-C4C-C3C	-4.34	118.30	124.97
23	C	506	CLA	C2D-C1D-ND	4.34	114.51	109.56
23	C	509	CLA	C1D-C2D-C3D	-4.34	102.72	106.97
25	d	404	BCR	C15-C14-C13	-4.33	121.03	127.29
23	C	513	CLA	CBD-CHA-C1A	4.33	134.43	128.77
23	A	407	CLA	C4B-C3B-CAB	-4.33	118.41	127.18
23	b	615	CLA	C3B-C4B-CHC	-4.32	117.80	126.00
23	B	609	CLA	C1C-C2C-C3C	-4.32	101.52	106.96
23	A	405	CLA	C2C-C1C-NC	4.32	113.71	110.22
23	C	503	CLA	C3B-CAB-CBB	-4.32	117.01	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C3B-C4B-CHC	-4.32	117.81	126.00
23	c	910	CLA	C3B-C2B-C1B	-4.31	101.91	106.69
26	D	407	SQD	C1-O5-C5	-4.31	105.39	113.73
23	B	609	CLA	C3B-C4B-CHC	-4.31	117.83	126.00
23	c	902	CLA	CHD-C4C-C3C	-4.31	118.36	124.97
23	c	914	CLA	C2C-C1C-NC	4.30	113.70	110.22
34	h	102	DGD	C3E-C4E-C5E	-4.30	102.44	110.17
23	c	908	CLA	C3B-C4B-CHC	-4.30	117.85	126.00
23	C	513	CLA	C3B-C2B-C1B	-4.30	101.93	106.69
34	c	917	DGD	O3G-C3G-C2G	-4.29	100.77	110.99
23	b	606	CLA	C1C-C2C-C3C	-4.29	101.56	106.96
23	b	614	CLA	CBD-CHA-C1A	4.29	134.38	128.77
25	t	101	BCR	C11-C10-C9	-4.29	121.09	127.29
23	b	615	CLA	C4C-C3C-C2C	-4.29	99.90	106.93
23	A	406	CLA	C3B-C4B-CHC	-4.28	117.88	126.00
23	a	410	CLA	C3B-C2B-C1B	-4.28	101.94	106.69
23	b	618	CLA	C1C-C2C-C3C	-4.28	101.58	106.96
23	b	611	CLA	O2D-CGD-CBD	4.28	119.98	111.34
23	d	402	CLA	C1C-C2C-C3C	-4.27	101.59	106.96
23	C	504	CLA	C3B-CAB-CBB	-4.27	117.11	125.95
25	D	404	BCR	C40-C30-C25	-4.26	103.27	110.33
24	a	412	PHO	O2D-CGD-CBD	4.26	119.95	111.34
23	c	905	CLA	C4B-C3B-C2B	-4.26	102.66	107.04
23	c	909	CLA	CMD-C2D-C3D	4.26	133.19	125.16
23	c	906	CLA	CBD-CHA-C1A	4.26	134.33	128.77
23	b	618	CLA	C2D-C1D-ND	4.26	114.41	109.56
23	b	617	CLA	C4-C3-C2	-4.25	115.05	123.52
23	b	607	CLA	C3B-C4B-CHC	-4.25	117.93	126.00
23	C	510	CLA	C4B-CHC-C1C	-4.25	121.88	127.47
23	C	513	CLA	O2D-CGD-CBD	4.25	119.92	111.34
23	b	616	CLA	C4B-CHC-C1C	-4.25	121.88	127.47
23	D	403	CLA	C3B-C4B-CHC	-4.25	117.94	126.00
23	B	607	CLA	O2D-CGD-O1D	-4.25	115.26	123.79
30	A	419	LMT	O2'-C2'-C1'	4.24	119.26	110.03
26	D	407	SQD	O47-C7-C8	4.24	120.58	111.54
23	b	611	CLA	C2D-C1D-ND	4.24	114.40	109.56
23	A	410	CLA	C4D-ND-C1D	-4.24	101.44	106.57
23	b	617	CLA	CHD-C4C-C3C	-4.23	118.47	124.97
23	B	606	CLA	CHD-C4C-C3C	-4.23	118.47	124.97
23	C	503	CLA	CMB-C2B-C3B	4.23	133.14	125.16
23	a	411	CLA	C2A-C1A-NA	4.23	116.74	111.33
33	c	923	HTG	C2-C1-S1	-4.22	106.22	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	C3C-C4C-NC	4.22	115.24	110.15
23	b	612	CLA	C3B-CAB-CBB	-4.22	117.21	125.95
23	B	615	CLA	C4-C3-C5	4.22	121.80	115.39
23	C	512	CLA	C2D-C1D-ND	4.22	114.37	109.56
23	b	611	CLA	C4B-C3B-C2B	-4.22	102.71	107.04
23	b	605	CLA	O2D-CGD-O1D	-4.22	115.32	123.79
30	b	624	LMT	O5'-C5'-C4'	4.22	118.55	109.71
23	C	512	CLA	C1-C2-C3	-4.21	118.92	126.23
23	B	606	CLA	C3B-C4B-CHC	-4.21	118.02	126.00
23	B	603	CLA	C2C-C1C-NC	4.21	113.62	110.22
23	B	617	CLA	C3B-C4B-CHC	-4.21	118.02	126.00
23	b	617	CLA	C4D-ND-C1D	-4.21	101.49	106.57
23	B	616	CLA	C2D-C1D-ND	4.20	114.36	109.56
23	c	905	CLA	CHD-C4C-NC	4.20	127.22	124.28
36	d	407	LHG	O8-C23-O10	-4.19	112.52	123.48
23	b	614	CLA	CHD-C4C-C3C	-4.19	118.53	124.97
23	d	403	CLA	C3B-C4B-CHC	-4.19	118.05	126.00
27	b	623	LMG	O7-C10-C11	4.19	120.46	111.54
23	C	501	CLA	C2D-C1D-ND	4.19	114.33	109.56
23	A	407	CLA	C3B-C2B-C1B	-4.18	102.05	106.69
23	c	910	CLA	C2D-C1D-ND	4.18	114.33	109.56
23	C	504	CLA	C4-C3-C5	4.18	121.74	115.39
23	d	403	CLA	C3B-CAB-CBB	-4.18	117.30	125.95
23	b	618	CLA	CMB-C2B-C3B	4.17	133.03	125.16
25	K	102	BCR	C7-C8-C9	-4.17	119.97	126.22
23	A	407	CLA	O2D-CGD-CBD	4.17	119.77	111.34
23	C	508	CLA	C2D-C1D-ND	4.17	114.31	109.56
23	B	610	CLA	C2D-C1D-ND	4.17	114.32	109.56
23	a	411	CLA	C4-C3-C5	4.17	121.72	115.39
23	B	612	CLA	O2D-CGD-O1D	-4.17	115.42	123.79
23	C	509	CLA	C1C-C2C-C3C	-4.17	101.72	106.96
23	C	504	CLA	C4B-C3B-C2B	-4.16	102.77	107.04
34	C	518	DGD	O3G-C3G-C2G	-4.16	101.10	110.99
26	a	401	SQD	O47-C7-C8	4.16	120.40	111.54
23	B	612	CLA	O2D-CGD-CBD	4.15	119.73	111.34
23	b	607	CLA	C3C-C4C-NC	4.15	115.15	110.15
23	B	617	CLA	C3C-C4C-NC	4.15	115.15	110.15
23	D	403	CLA	C3B-C2B-C1B	-4.14	102.09	106.69
23	c	913	CLA	C3B-CAB-CBB	-4.14	117.37	125.95
23	c	913	CLA	C2D-C1D-ND	4.14	114.29	109.56
23	c	908	CLA	C4-C3-C5	4.14	121.68	115.39
23	c	909	CLA	C2C-C1C-NC	4.14	113.57	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C2D-C1D-ND	4.14	114.28	109.56
23	c	907	CLA	C2C-C1C-NC	4.14	113.57	110.22
23	A	407	CLA	CMC-C2C-C1C	4.14	130.85	124.95
23	b	606	CLA	C3B-CAB-CBB	-4.14	117.39	125.95
23	B	608	CLA	C3B-C4B-NB	4.13	114.55	109.21
24	A	408	PHO	CMD-C2D-C1D	4.13	134.79	128.49
23	A	405	CLA	C1D-CHD-C4C	-4.13	116.20	122.60
28	a	419	PL9	C25-C24-C26	4.13	121.66	115.39
23	B	605	CLA	C2B-C1B-NB	4.13	112.25	109.50
23	b	607	CLA	C1C-C2C-C3C	-4.12	101.77	106.96
23	c	907	CLA	CMC-C2C-C1C	4.13	130.83	124.95
23	C	509	CLA	C4B-CHC-C1C	-4.12	122.04	127.47
25	d	404	BCR	C24-C23-C22	-4.12	120.05	126.22
24	a	413	PHO	C2D-C1D-ND	4.12	116.27	107.96
28	d	405	PL9	C15-C14-C16	4.12	121.64	115.39
27	C	519	LMG	O7-C10-C11	4.12	120.31	111.54
26	B	621	SQD	O48-C23-C24	4.12	124.50	111.90
23	B	606	CLA	C2A-C1A-NA	4.12	116.60	111.33
23	c	904	CLA	C2D-C1D-ND	4.11	114.25	109.56
23	b	618	CLA	CBD-CHA-C1A	4.11	134.14	128.77
23	c	908	CLA	C2D-C1D-ND	4.11	114.25	109.56
23	B	603	CLA	C4-C3-C5	4.11	121.62	115.39
23	c	907	CLA	CHB-C4A-NA	4.11	130.11	124.38
27	B	622	LMG	O7-C10-O9	-4.11	112.70	123.66
28	a	419	PL9	C37-C38-C39	-4.10	118.94	127.81
24	A	408	PHO	C4D-ND-C1D	-4.10	99.58	108.62
23	b	614	CLA	C1-C2-C3	-4.10	119.12	126.23
23	b	607	CLA	CMC-C2C-C1C	4.09	130.79	124.95
23	C	512	CLA	C4-C3-C5	4.09	121.61	115.39
23	B	605	CLA	C3B-C4B-CHC	-4.09	118.24	126.00
23	b	607	CLA	C3B-CAB-CBB	-4.09	117.48	125.95
25	K	101	BCR	C38-C26-C25	-4.09	119.88	124.50
25	d	404	BCR	C38-C26-C25	-4.09	119.88	124.50
25	c	915	BCR	C33-C5-C6	-4.08	119.88	124.50
23	d	403	CLA	C4-C3-C5	4.09	121.59	115.39
23	a	410	CLA	C4B-CHC-C1C	-4.09	122.09	127.47
23	B	604	CLA	C2D-C1D-ND	4.08	114.21	109.56
23	b	607	CLA	CAC-C3C-C4C	4.08	130.97	124.85
23	c	911	CLA	C3B-C4B-CHC	-4.08	118.27	126.00
23	A	407	CLA	CMB-C2B-C3B	4.08	132.85	125.16
23	c	904	CLA	C3B-CAB-CBB	-4.08	117.51	125.95
34	C	516	DGD	O3G-C3G-C2G	-4.08	101.29	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	BCR	C29-C30-C25	4.07	116.87	110.37
23	b	605	CLA	O2D-CGD-CBD	4.07	119.57	111.34
23	D	403	CLA	CED-O2D-CGD	4.07	125.69	116.00
23	B	615	CLA	C3B-C4B-CHC	-4.06	118.29	126.00
23	B	603	CLA	C2B-C1B-NB	4.06	112.21	109.50
23	c	902	CLA	O2D-CGD-CBD	4.06	119.55	111.34
30	a	402	LMT	C1-O1'-C1'	4.05	121.06	113.91
23	A	405	CLA	CAC-C3C-C4C	4.05	130.93	124.85
34	H	102	DGD	O1G-C1A-O1A	-4.05	112.90	123.48
23	C	511	CLA	C3B-C4B-NB	4.04	114.44	109.21
27	c	920	LMG	O7-C10-C11	4.04	120.15	111.54
23	b	611	CLA	C1C-C2C-C3C	-4.04	101.88	106.96
23	b	612	CLA	CBD-CHA-C1A	4.04	134.04	128.77
23	c	912	CLA	O2D-CGD-O1D	-4.04	115.69	123.79
23	B	612	CLA	C3B-C2B-C1B	-4.03	102.22	106.69
36	d	407	LHG	O8-C23-C24	4.03	124.24	111.90
23	b	609	CLA	C4A-NA-C1A	4.03	112.06	106.38
23	a	411	CLA	C1C-C2C-C3C	-4.03	101.89	106.96
23	B	610	CLA	C4B-C3B-CAB	-4.03	119.02	127.18
23	C	505	CLA	C3B-C4B-CHC	-4.02	118.38	126.00
23	b	618	CLA	C1D-CHD-C4C	-4.02	116.37	122.60
23	C	502	CLA	C3B-CAB-CBB	-4.02	117.63	125.95
23	C	502	CLA	CAC-C3C-C4C	4.02	130.88	124.85
26	A	412	SQD	C45-O47-C7	-4.02	108.42	117.86
23	C	507	CLA	CBC-CAC-C3C	-4.02	100.21	112.37
23	d	402	CLA	C3B-C4B-NB	4.00	114.38	109.21
23	d	403	CLA	C4B-CHC-C1C	-4.00	122.21	127.47
23	B	616	CLA	C3B-C4B-CHC	-4.00	118.42	126.00
23	b	610	CLA	CAC-C3C-C4C	4.00	130.85	124.85
23	a	410	CLA	C1D-CHD-C4C	-4.00	116.40	122.60
23	C	511	CLA	CHD-C4C-C3C	-4.00	118.83	124.97
23	B	610	CLA	C2B-C3B-CAB	4.00	135.50	127.33
23	B	612	CLA	CMD-C2D-C3D	3.99	132.69	125.16
23	b	618	CLA	CHD-C4C-C3C	-3.99	118.84	124.97
23	b	616	CLA	C3B-C4B-CHC	-3.99	118.43	126.00
23	A	407	CLA	C4-C3-C5	3.99	121.45	115.39
23	B	607	CLA	CMD-C2D-C1D	3.99	134.05	126.16
23	A	406	CLA	CGD-CBD-CHA	-3.99	104.40	113.65
36	L	101	LHG	O7-C7-O9	-3.99	113.03	123.66
23	c	906	CLA	C2D-C1D-ND	3.99	114.11	109.56
23	d	402	CLA	CMD-C2D-C3D	3.98	132.66	125.16
23	b	604	CLA	CBD-CHA-C1A	3.98	133.97	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	CHD-C4C-NC	3.98	127.06	124.28
23	B	602	CLA	C3B-C2B-C1B	-3.97	102.28	106.69
23	c	911	CLA	CHD-C4C-NC	3.97	127.06	124.28
23	a	410	CLA	C3B-CAB-CBB	-3.97	117.72	125.95
23	B	611	CLA	CAA-CBA-CGA	-3.97	101.53	113.24
23	C	508	CLA	CGD-CBD-CHA	-3.97	104.44	113.65
23	A	406	CLA	C3B-C2B-C1B	-3.97	102.29	106.69
23	B	606	CLA	CHD-C4C-NC	3.97	127.06	124.28
23	b	612	CLA	O2D-CGD-CBD	3.97	119.36	111.34
23	c	912	CLA	C3B-CAB-CBB	-3.97	117.73	125.95
23	c	906	CLA	CMB-C2B-C3B	3.97	132.64	125.16
23	b	604	CLA	C2D-C1D-ND	3.97	114.09	109.56
23	C	504	CLA	C3B-C4B-CHC	-3.97	118.48	126.00
23	b	614	CLA	C2D-C1D-ND	3.96	114.08	109.56
23	b	606	CLA	CMB-C2B-C3B	3.96	132.63	125.16
23	C	512	CLA	O2D-CGD-CBD	3.96	119.34	111.34
27	c	921	LMG	O7-C10-C11	3.96	119.97	111.54
23	b	619	CLA	C2B-C3B-CAB	3.96	135.42	127.33
23	C	508	CLA	C4-C3-C5	3.96	121.40	115.39
23	c	904	CLA	C1-C2-C3	-3.96	119.36	126.23
23	C	502	CLA	C3B-C2B-C1B	-3.96	102.31	106.69
23	c	911	CLA	C4-C3-C5	3.95	121.39	115.39
23	A	406	CLA	C3B-CAB-CBB	-3.95	117.77	125.95
23	C	513	CLA	C2C-C1C-NC	3.95	113.41	110.22
23	B	612	CLA	C2D-C1D-ND	3.95	114.06	109.56
23	c	912	CLA	C1C-C2C-C3C	-3.95	101.99	106.96
24	a	413	PHO	C4-C3-C5	3.95	121.38	115.39
27	b	623	LMG	O8-C28-O10	-3.94	113.17	123.48
23	b	618	CLA	CMC-C2C-C1C	3.94	130.57	124.95
23	C	505	CLA	C3B-C2B-C1B	-3.94	102.32	106.69
30	A	419	LMT	C1'-O5'-C5'	3.94	121.36	113.73
23	B	606	CLA	C2B-C3B-CAB	3.94	135.38	127.33
23	B	606	CLA	CGD-CBD-CHA	-3.94	104.52	113.65
23	A	406	CLA	C4B-CHC-C1C	-3.94	122.29	127.47
23	A	407	CLA	C1C-C2C-C3C	-3.94	102.01	106.96
23	A	410	CLA	C3B-C2B-C1B	-3.93	102.33	106.69
23	c	914	CLA	C3B-CAB-CBB	-3.93	117.81	125.95
23	B	606	CLA	C4B-C3B-CAB	-3.93	119.22	127.18
34	C	518	DGD	O2G-C1B-C2B	3.93	119.91	111.54
24	a	412	PHO	CMB-C2B-C3B	3.93	132.56	125.16
23	C	505	CLA	CMD-C2D-C3D	3.92	132.56	125.16
34	C	516	DGD	O2G-C1B-C2B	3.93	119.90	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C2D-C1D-ND	3.92	114.03	109.56
25	D	404	BCR	C24-C23-C22	-3.92	120.34	126.22
23	c	903	CLA	C1D-CHD-C4C	-3.92	116.52	122.60
23	a	414	CLA	C4-C3-C5	3.92	121.34	115.39
23	b	618	CLA	O2D-CGD-O1D	-3.91	115.93	123.79
25	T	101	BCR	C20-C21-C22	-3.91	121.63	127.29
24	a	412	PHO	C2D-C1D-ND	3.91	115.86	107.96
23	D	403	CLA	C4B-CHC-C1C	-3.91	122.32	127.47
23	a	410	CLA	CMD-C2D-C3D	3.91	132.53	125.16
23	b	619	CLA	O2A-CGA-CBA	3.91	123.85	111.90
23	c	904	CLA	C3B-C2B-C1B	-3.90	102.36	106.69
23	b	610	CLA	C4B-CHC-C1C	-3.90	122.34	127.47
23	b	619	CLA	C4B-C3B-CAB	-3.90	119.28	127.18
23	b	608	CLA	O2D-CGD-CBD	3.90	119.21	111.34
23	b	606	CLA	CMC-C2C-C1C	3.90	130.51	124.95
23	b	613	CLA	C1C-C2C-C3C	-3.90	102.06	106.96
24	a	412	PHO	CBA-CAA-C2A	-3.90	104.42	113.95
26	D	407	SQD	C44-O6-C1	-3.88	106.02	113.80
34	d	406	DGD	O2G-C1B-C2B	3.88	119.80	111.54
23	d	402	CLA	C4B-NB-C1B	-3.87	103.39	107.12
23	C	510	CLA	C2D-C1D-ND	3.87	113.98	109.56
23	B	603	CLA	C3B-C4B-CHC	-3.87	118.66	126.00
23	B	615	CLA	C3B-C2B-C1B	-3.87	102.40	106.69
23	b	604	CLA	C3B-C2B-C1B	-3.87	102.40	106.69
23	D	402	CLA	C3B-CAB-CBB	-3.86	117.95	125.95
23	b	612	CLA	C3C-C4C-NC	3.86	114.81	110.15
23	C	512	CLA	C3B-C2B-C1B	-3.86	102.41	106.69
23	d	403	CLA	C1C-C2C-C3C	-3.85	102.11	106.96
23	d	403	CLA	CHD-C4C-C3C	-3.85	119.05	124.97
23	b	607	CLA	O2D-CGD-O1D	-3.85	116.05	123.79
24	A	408	PHO	CHD-C4C-NC	-3.85	121.80	128.68
23	B	608	CLA	CMD-C2D-C3D	3.85	132.43	125.16
25	t	101	BCR	C28-C27-C26	-3.85	107.48	113.81
23	B	612	CLA	C1D-CHD-C4C	-3.85	116.63	122.60
25	B	618	BCR	C33-C5-C6	-3.84	120.16	124.50
26	A	418	SQD	O47-C7-C8	3.84	119.72	111.54
24	a	412	PHO	C4C-C3C-C2C	-3.84	102.38	106.83
23	c	904	CLA	CMD-C2D-C3D	3.84	132.39	125.16
23	B	615	CLA	O2D-CGD-CBD	3.84	119.09	111.34
23	C	508	CLA	O2D-CGD-CBD	3.83	119.07	111.34
30	B	623	LMT	C1B-O5B-C5B	3.83	121.13	113.73
23	b	611	CLA	O2D-CGD-O1D	-3.83	116.11	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C3B-C2B-C1B	-3.82	102.45	106.69
27	C	519	LMG	O8-C28-C29	3.82	123.60	111.90
23	d	403	CLA	C3B-C4B-NB	3.82	114.15	109.21
23	C	513	CLA	C3B-C4B-CHC	-3.82	118.76	126.00
23	c	902	CLA	C4D-ND-C1D	-3.82	101.96	106.57
23	a	414	CLA	C3C-C4C-NC	3.82	114.75	110.15
23	b	615	CLA	C1-C2-C3	-3.81	119.62	126.23
30	c	922	LMT	O1'-C1'-C2'	3.80	113.02	108.15
23	B	608	CLA	C4B-NB-C1B	-3.80	103.46	107.12
23	B	615	CLA	O2D-CGD-O1D	-3.80	116.16	123.79
23	b	614	CLA	C3B-C4B-CHC	-3.79	118.81	126.00
23	C	503	CLA	C3B-C4B-CHC	-3.79	118.81	126.00
23	d	402	CLA	C4B-C3B-C2B	-3.79	103.14	107.04
23	C	513	CLA	CHD-C4C-C3C	-3.79	119.15	124.97
38	H	101	RRX	C7-C8-C9	-3.79	120.55	126.22
23	D	402	CLA	C3B-C4B-CHC	-3.79	118.82	126.00
23	a	409	CLA	C3B-C4B-CHC	-3.78	118.82	126.00
23	c	905	CLA	C4D-ND-C1D	-3.79	101.99	106.57
33	b	601	HTG	C1'-S1-C1	3.78	105.68	100.19
23	A	406	CLA	O2D-CGD-CBD	3.78	118.98	111.34
23	C	502	CLA	C2A-C1A-NA	3.78	116.17	111.33
24	a	413	PHO	C4D-ND-C1D	-3.78	100.29	108.62
23	b	604	CLA	CMD-C2D-C3D	3.78	132.28	125.16
23	B	616	CLA	C3C-C4C-NC	3.78	114.70	110.15
23	d	402	CLA	CHC-C4B-NB	3.77	131.11	124.70
23	c	908	CLA	C4B-C3B-CAB	-3.77	119.53	127.18
23	B	602	CLA	C3B-C4B-CHC	-3.77	118.85	126.00
23	C	511	CLA	O2D-CGD-CBD	3.77	118.96	111.34
23	a	414	CLA	C3B-C4B-NB	3.77	114.08	109.21
23	C	506	CLA	CHC-C4B-NB	3.77	131.10	124.70
30	m	101	LMT	C3'-C4'-C5'	-3.76	102.44	110.86
36	a	417	LHG	O7-C7-C8	3.76	119.56	111.54
23	a	411	CLA	C3B-C4B-CHC	-3.76	118.88	126.00
33	V	202	HTG	O2-C2-C1	3.76	116.39	110.13
23	c	912	CLA	O2D-CGD-CBD	3.76	118.93	111.34
24	A	409	PHO	C4D-ND-C1D	-3.75	100.35	108.62
23	B	617	CLA	C4B-C3B-CAB	-3.75	119.58	127.18
23	a	414	CLA	C3B-CAB-CBB	-3.75	118.18	125.95
24	A	408	PHO	CAC-C3C-C4C	3.75	129.71	125.18
23	b	612	CLA	C3B-C2B-C1B	-3.74	102.54	106.69
23	c	909	CLA	C3B-C2B-C1B	-3.74	102.54	106.69
30	F	102	LMT	C1B-O5B-C5B	3.74	120.97	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	501	CLA	C3B-CAB-CBB	-3.74	118.20	125.95
28	d	405	PL9	C40-C39-C38	-3.74	116.08	123.52
23	b	605	CLA	C3B-CAB-CBB	-3.74	118.21	125.95
23	a	410	CLA	CBD-CHA-C1A	3.74	133.66	128.77
23	C	506	CLA	C3B-C2B-C1B	-3.74	102.55	106.69
23	b	606	CLA	C2B-C3B-CAB	3.73	134.96	127.33
23	C	510	CLA	C2B-C3B-CAB	3.73	134.96	127.33
25	B	618	BCR	C15-C14-C13	-3.73	121.90	127.29
23	b	618	CLA	CHC-C4B-NB	3.73	131.03	124.70
23	b	614	CLA	C1C-C2C-C3C	-3.72	102.28	106.96
23	B	608	CLA	C3B-CAB-CBB	-3.72	118.25	125.95
23	C	510	CLA	C3B-C4B-NB	3.71	114.01	109.21
23	C	508	CLA	C1C-C2C-C3C	-3.71	102.29	106.96
23	A	407	CLA	C4B-C3B-C2B	-3.71	103.22	107.04
23	A	405	CLA	C3B-C2B-C1B	-3.71	102.58	106.69
25	D	404	BCR	C38-C26-C25	-3.71	120.31	124.50
23	D	403	CLA	C1C-C2C-C3C	-3.71	102.29	106.96
23	C	502	CLA	C3B-C4B-CHC	-3.71	118.97	126.00
23	B	605	CLA	CED-O2D-CGD	3.71	124.83	116.00
23	D	402	CLA	CAC-C3C-C4C	3.70	130.41	124.85
28	D	405	PL9	C27-C28-C29	-3.70	119.81	127.81
25	d	404	BCR	C16-C15-C14	-3.70	115.30	123.45
23	a	414	CLA	O2D-CGD-CBD	3.70	118.81	111.34
23	C	512	CLA	C1-O2A-CGA	3.70	127.75	117.00
23	b	614	CLA	C3B-C4B-NB	3.70	113.99	109.21
27	Z	101	LMG	C9-C8-C7	-3.69	103.38	111.86
23	c	908	CLA	C4B-CHC-C1C	-3.69	122.61	127.47
23	B	612	CLA	C3B-CAB-CBB	-3.69	118.31	125.95
23	C	503	CLA	C2D-C1D-ND	3.69	113.77	109.56
30	b	625	LMT	C3'-C4'-C5'	-3.69	104.61	110.58
23	b	605	CLA	CBD-CHA-C1A	3.69	133.59	128.77
23	b	607	CLA	C6-C5-C3	-3.69	104.21	112.62
23	b	615	CLA	O2D-CGD-O1D	-3.68	116.39	123.79
23	B	616	CLA	CBD-CHA-C1A	3.68	133.58	128.77
23	b	605	CLA	CHD-C4C-C3C	-3.68	119.32	124.97
23	C	507	CLA	C4B-C3B-CAB	-3.68	119.73	127.18
23	c	907	CLA	CMD-C2D-C1D	3.68	133.43	126.16
23	b	616	CLA	C4B-C3B-C2B	-3.68	103.26	107.04
23	a	411	CLA	C2B-C1B-CHB	-3.67	119.04	126.00
23	B	612	CLA	C1-C2-C3	-3.67	119.86	126.23
23	C	506	CLA	C1C-C2C-C3C	-3.67	102.34	106.96
23	c	912	CLA	C2D-C1D-ND	3.67	113.75	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	C4-C3-C5	3.67	120.96	115.39
23	A	407	CLA	C3B-C4B-NB	3.67	113.95	109.21
33	B	624	HTG	C1'-S1-C1	3.67	105.52	100.19
23	c	905	CLA	C3B-C4B-CHC	-3.67	119.04	126.00
23	B	603	CLA	C2D-C1D-ND	3.67	113.74	109.56
23	c	913	CLA	C1-O2A-CGA	3.67	127.66	117.00
23	b	613	CLA	CHD-C4C-C3C	-3.66	119.34	124.97
23	B	608	CLA	C2A-C1A-NA	3.66	116.02	111.33
23	B	609	CLA	O2D-CGD-O1D	-3.66	116.44	123.79
23	C	505	CLA	C2B-C3B-CAB	3.66	134.81	127.33
30	F	102	LMT	O4'-C4B-C5B	3.66	118.94	109.25
23	C	501	CLA	C1C-C2C-C3C	-3.66	102.36	106.96
23	b	606	CLA	C5-C3-C2	-3.66	114.03	121.06
23	B	609	CLA	C4B-C3B-C2B	-3.66	103.28	107.04
34	c	919	DGD	C6B-C5B-C4B	-3.65	95.15	114.56
23	B	609	CLA	C3B-C2B-C1B	-3.65	102.64	106.69
23	B	608	CLA	C3B-C4B-CHC	-3.65	119.07	126.00
25	b	622	BCR	C24-C23-C22	-3.65	120.75	126.22
23	b	618	CLA	O2D-CGD-CBD	3.65	118.71	111.34
23	a	414	CLA	CHC-C4B-NB	3.64	130.89	124.70
23	B	617	CLA	CMD-C2D-C3D	3.64	132.03	125.16
23	B	611	CLA	O2D-CGD-O1D	-3.64	116.47	123.79
23	B	616	CLA	C3B-CAB-CBB	-3.64	118.41	125.95
25	a	415	BCR	C28-C27-C26	-3.64	107.83	113.81
23	a	414	CLA	CMD-C2D-C3D	3.64	132.02	125.16
23	c	910	CLA	C4-C3-C5	3.64	120.92	115.39
30	M	102	LMT	C1'-O5'-C5'	-3.64	106.69	113.73
23	C	511	CLA	C4B-NB-C1B	-3.64	103.62	107.12
23	B	610	CLA	C1-C2-C3	-3.64	119.92	126.23
27	c	920	LMG	O8-C28-C29	3.63	123.03	111.90
28	D	405	PL9	C40-C39-C38	-3.63	116.29	123.52
23	b	619	CLA	CMB-C2B-C3B	3.63	132.00	125.16
27	D	411	LMG	O8-C28-O10	-3.63	113.99	123.48
23	B	614	CLA	CMD-C2D-C1D	3.63	133.34	126.16
23	C	503	CLA	C1C-C2C-C3C	-3.63	102.40	106.96
25	D	404	BCR	C28-C27-C26	-3.63	107.85	113.81
23	b	610	CLA	C4-C3-C5	3.63	120.90	115.39
23	a	414	CLA	C1-C2-C3	-3.63	119.94	126.23
23	c	908	CLA	C2B-C3B-CAB	3.62	134.74	127.33
23	C	510	CLA	C3B-C2B-C1B	-3.62	102.67	106.69
23	c	904	CLA	CHD-C4C-C3C	-3.62	119.41	124.97
23	B	617	CLA	O2A-C1-C2	3.62	116.41	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	908	CLA	C1C-C2C-C3C	-3.61	102.41	106.96
23	c	904	CLA	C4A-NA-C1A	3.61	111.48	106.38
23	c	910	CLA	C3B-C4B-NB	3.61	113.88	109.21
23	D	402	CLA	C2D-C1D-ND	3.61	113.68	109.56
23	C	506	CLA	C3B-C4B-CHC	-3.61	119.15	126.00
23	B	602	CLA	O2D-CGD-O1D	-3.61	116.54	123.79
23	D	403	CLA	CBD-CHA-C1A	3.61	133.49	128.77
23	B	611	CLA	O2D-CGD-CBD	3.61	118.63	111.34
23	b	610	CLA	CBD-CHA-C1A	3.61	133.49	128.77
23	D	402	CLA	O2D-CGD-O1D	-3.61	116.55	123.79
23	A	405	CLA	C3B-C4B-NB	3.61	113.87	109.21
23	b	604	CLA	C4-C3-C5	3.61	120.87	115.39
23	b	618	CLA	C1B-CHB-C4A	-3.60	122.98	130.12
23	C	509	CLA	C3C-C4C-NC	3.60	114.49	110.15
24	A	409	PHO	C1-C2-C3	-3.60	119.99	126.23
23	C	507	CLA	C1C-C2C-C3C	-3.60	102.43	106.96
23	B	610	CLA	C3B-C4B-CHC	-3.59	119.18	126.00
23	c	910	CLA	CHC-C4B-NB	3.59	130.80	124.70
23	C	512	CLA	O2D-CGD-O1D	-3.59	116.58	123.79
23	d	402	CLA	OBD-CAD-C3D	-3.59	120.90	128.15
23	B	606	CLA	CBD-CHA-C1A	3.59	133.46	128.77
23	B	617	CLA	C2B-C3B-CAB	3.59	134.67	127.33
23	B	607	CLA	C3B-CAB-CBB	-3.59	118.52	125.95
30	m	101	LMT	O1'-C1'-C2'	3.58	112.75	108.15
23	b	604	CLA	C1C-C2C-C3C	-3.58	102.45	106.96
23	D	402	CLA	C4D-ND-C1D	3.58	110.89	106.57
23	b	606	CLA	CBD-CHA-C1A	3.58	133.45	128.77
23	b	613	CLA	C3B-C4B-CHC	-3.58	119.21	126.00
23	B	606	CLA	C3C-C4C-NC	3.58	114.47	110.15
23	C	505	CLA	C4B-CHC-C1C	-3.58	122.76	127.47
23	B	611	CLA	O2A-CGA-O1A	-3.58	114.12	123.48
28	d	405	PL9	C36-C37-C38	-3.58	101.47	111.64
23	B	602	CLA	C1C-C2C-C3C	-3.58	102.46	106.96
23	B	605	CLA	C1C-NC-C4C	-3.58	101.44	106.26
23	c	906	CLA	CAC-C3C-C4C	3.58	130.22	124.85
23	c	912	CLA	C4-C3-C5	3.57	120.82	115.39
23	C	503	CLA	C2B-C3B-CAB	3.57	134.64	127.33
23	C	509	CLA	CHD-C4C-C3C	-3.57	119.49	124.97
27	c	921	LMG	O1-C1-C2	3.57	112.72	108.15
23	D	402	CLA	C4B-C3B-C2B	-3.57	103.38	107.04
23	B	617	CLA	C4B-CHC-C1C	-3.57	122.78	127.47
23	B	615	CLA	C4B-CHC-C1C	-3.57	122.78	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	419	PL9	C20-C19-C21	3.56	120.80	115.39
23	c	904	CLA	C3B-C4B-CHC	-3.56	119.24	126.00
24	A	409	PHO	C4-C3-C5	3.56	120.80	115.39
23	B	608	CLA	CBC-CAC-C3C	-3.56	101.58	112.37
23	B	617	CLA	CHC-C4B-NB	3.56	130.75	124.70
23	C	503	CLA	C4B-C3B-CAB	-3.56	119.97	127.18
36	L	101	LHG	C6-C5-C4	-3.55	103.70	111.86
23	B	606	CLA	C4-C3-C5	3.56	120.79	115.39
24	A	409	PHO	CHD-C4C-NC	-3.55	122.34	128.68
23	a	414	CLA	C4B-C3B-C2B	-3.55	103.39	107.04
23	C	504	CLA	O2D-CGD-O1D	-3.55	116.66	123.79
23	B	612	CLA	CHC-C4B-NB	3.55	130.73	124.70
23	C	504	CLA	CBD-CHA-C1A	3.55	133.41	128.77
23	b	617	CLA	O2A-CGA-O1A	-3.54	114.22	123.48
23	a	409	CLA	C4B-CHC-C1C	-3.55	122.81	127.47
23	C	502	CLA	CGD-CBD-CHA	-3.55	105.43	113.65
23	C	511	CLA	O2D-CGD-O1D	-3.54	116.67	123.79
23	c	903	CLA	O2D-CGD-O1D	-3.54	116.68	123.79
23	C	506	CLA	C2B-C1B-NB	3.54	111.86	109.50
23	A	405	CLA	CHD-C4C-C3C	-3.54	119.53	124.97
23	B	607	CLA	C1C-C2C-C3C	-3.54	102.51	106.96
36	d	407	LHG	C6-O8-C23	3.53	127.08	116.99
23	B	613	CLA	CHD-C4C-C3C	-3.53	119.54	124.97
30	J	102	LMT	C3'-C4'-C5'	-3.53	104.87	110.58
23	a	414	CLA	CMC-C2C-C1C	3.53	129.98	124.95
23	C	507	CLA	C3B-CAB-CBB	-3.52	118.65	125.95
23	C	507	CLA	C4-C3-C5	3.52	120.74	115.39
23	b	604	CLA	O2A-CGA-CBA	3.53	122.69	111.90
23	b	619	CLA	C4B-CHC-C1C	-3.52	122.84	127.47
23	b	605	CLA	C3A-C4A-NA	3.52	115.07	110.81
23	A	410	CLA	CHB-C4A-NA	3.52	129.29	124.38
27	b	623	LMG	O7-C10-O9	-3.52	114.28	123.66
23	c	911	CLA	CGD-CBD-CHA	-3.51	105.50	113.65
23	c	906	CLA	CBC-CAC-C3C	-3.51	101.73	112.37
34	H	102	DGD	O1G-C1A-C2A	3.51	122.65	111.90
26	a	416	SQD	O8-S-C6	3.51	110.07	105.89
28	d	405	PL9	C22-C23-C24	-3.50	120.23	127.81
23	a	414	CLA	C1C-C2C-C3C	-3.50	102.55	106.96
24	a	413	PHO	C4C-C3C-C2C	-3.50	102.77	106.83
23	B	609	CLA	CMD-C2D-C3D	3.50	131.76	125.16
23	B	602	CLA	CMC-C2C-C1C	3.50	129.94	124.95
23	c	905	CLA	CHD-C4C-C3C	-3.50	119.59	124.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C2B-C3B-CAB	3.50	134.48	127.33
23	b	612	CLA	CHD-C4C-C3C	-3.50	119.60	124.97
23	c	911	CLA	CHD-C4C-C3C	-3.50	119.60	124.97
23	b	619	CLA	O1D-CGD-CBD	-3.50	117.31	124.45
26	D	407	SQD	C6-C5-C4	3.49	119.23	111.86
23	C	511	CLA	C1C-C2C-C3C	-3.49	102.57	106.96
23	c	914	CLA	CMC-C2C-C1C	3.49	129.92	124.95
23	b	617	CLA	C3B-CAB-CBB	-3.49	118.73	125.95
23	b	609	CLA	C3B-C2B-C1B	-3.49	102.82	106.69
23	C	513	CLA	C1C-C2C-C3C	-3.49	102.57	106.96
23	B	604	CLA	C6-C5-C3	3.49	120.58	112.62
23	B	616	CLA	C11-C10-C8	-3.49	104.60	115.44
23	B	602	CLA	C3B-CAB-CBB	-3.49	118.73	125.95
23	c	902	CLA	C3B-C4B-NB	3.48	113.72	109.21
23	B	616	CLA	C1C-C2C-C3C	-3.48	102.58	106.96
23	C	506	CLA	CMC-C2C-C1C	3.48	129.91	124.95
23	C	513	CLA	O2D-CGD-O1D	-3.48	116.80	123.79
23	b	608	CLA	C1C-C2C-C3C	-3.48	102.58	106.96
23	C	513	CLA	C2B-C3B-CAB	3.48	134.44	127.33
23	B	602	CLA	C1-O2A-CGA	3.48	127.11	117.00
23	c	907	CLA	CHB-C1B-NB	-3.48	118.80	124.70
23	b	607	CLA	CHD-C4C-NC	3.47	126.71	124.28
23	D	402	CLA	C2A-C1A-NA	3.47	115.78	111.33
23	A	407	CLA	C2D-C1D-ND	3.47	113.52	109.56
23	B	607	CLA	C4B-C3B-C2B	-3.47	103.47	107.04
23	b	618	CLA	C4-C3-C5	3.47	120.66	115.39
23	B	606	CLA	O2A-CGA-O1A	-3.47	114.41	123.48
23	b	607	CLA	O2D-CGD-CBD	3.47	118.35	111.34
23	b	606	CLA	CMD-C2D-C3D	3.47	131.70	125.16
23	B	608	CLA	CBD-CHA-C1A	3.47	133.30	128.77
25	T	101	BCR	C35-C13-C12	3.46	123.69	118.09
23	c	907	CLA	C3A-C4A-CHB	-3.46	117.13	124.33
23	A	405	CLA	C3B-CAB-CBB	-3.46	118.78	125.95
23	c	905	CLA	C3B-C4B-NB	3.46	113.69	109.21
23	B	609	CLA	CAC-C3C-C4C	3.46	130.04	124.85
23	c	910	CLA	C3C-C4C-NC	3.46	114.32	110.15
25	b	620	BCR	C11-C10-C9	-3.46	122.29	127.29
23	c	902	CLA	C4A-NA-C1A	3.46	111.25	106.38
23	B	606	CLA	CMD-C2D-C3D	3.45	131.67	125.16
23	b	611	CLA	C3B-C2B-C1B	-3.45	102.86	106.69
23	c	902	CLA	C2B-C3B-CAB	3.45	134.39	127.33
23	B	608	CLA	CHD-C4C-C3C	-3.45	119.67	124.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	CAC-C3C-C4C	3.45	130.03	124.85
23	B	611	CLA	C4B-C3B-C2B	-3.45	103.50	107.04
30	C	520	LMT	C2'-C3'-C4'	-3.45	102.11	109.59
23	A	407	CLA	O2D-CGD-O1D	-3.45	116.87	123.79
23	C	507	CLA	C2D-C1D-ND	3.44	113.49	109.56
23	c	906	CLA	O2D-CGD-CBD	3.44	118.30	111.34
23	d	403	CLA	O1D-CGD-CBD	-3.44	117.42	124.45
23	A	410	CLA	C1C-C2C-C3C	-3.44	102.63	106.96
23	B	605	CLA	CAA-C2A-C3A	-3.44	104.70	113.32
23	C	507	CLA	C4A-NA-C1A	3.44	111.23	106.38
23	c	905	CLA	C4-C3-C5	3.44	120.62	115.39
23	B	602	CLA	C4A-NA-C1A	3.44	111.23	106.38
23	B	613	CLA	CBD-CHA-C1A	3.44	133.26	128.77
25	t	101	BCR	C38-C26-C25	-3.44	120.62	124.50
23	b	612	CLA	C1-C2-C3	-3.43	120.27	126.23
23	c	912	CLA	C1D-CHD-C4C	-3.43	117.28	122.60
23	b	605	CLA	C1C-C2C-C3C	-3.43	102.64	106.96
23	c	903	CLA	C1-C2-C3	-3.43	120.27	126.23
23	A	406	CLA	C3A-C4A-NA	3.43	114.96	110.81
23	B	613	CLA	CHC-C4B-NB	3.43	130.53	124.70
36	E	101	LHG	O7-C7-C8	3.43	118.85	111.54
25	K	102	BCR	C24-C23-C22	-3.43	121.08	126.22
28	A	414	PL9	C22-C23-C24	-3.43	120.39	127.81
23	c	912	CLA	C4A-NA-C1A	3.43	111.22	106.38
25	B	620	BCR	C15-C14-C13	-3.43	122.33	127.29
23	B	612	CLA	C1C-C2C-C3C	-3.43	102.65	106.96
23	B	616	CLA	CMD-C2D-C3D	3.43	131.62	125.16
23	B	610	CLA	C3C-C4C-NC	3.42	114.28	110.15
23	B	612	CLA	C3C-C4C-NC	3.42	114.28	110.15
26	B	621	SQD	C6-C5-C4	3.42	119.09	111.86
30	F	102	LMT	C2'-C3'-C4'	3.42	117.01	109.59
23	b	612	CLA	C3B-C4B-CHC	-3.42	119.51	126.00
23	B	605	CLA	O2D-CGD-CBD	3.42	118.25	111.34
26	a	401	SQD	O48-C23-C24	3.42	122.37	111.90
23	a	410	CLA	C2B-C3B-CAB	3.42	134.32	127.33
23	C	510	CLA	C4B-C3B-C2B	-3.42	103.53	107.04
23	C	501	CLA	C3B-C2B-C1B	-3.42	102.90	106.69
23	A	405	CLA	C4B-NB-C1B	-3.42	103.83	107.12
26	L	103	SQD	O47-C7-C8	3.42	118.82	111.54
23	c	905	CLA	C1C-C2C-C3C	-3.42	102.66	106.96
23	A	405	CLA	CMB-C2B-C3B	3.41	131.59	125.16
23	b	604	CLA	CMC-C2C-C1C	3.41	129.82	124.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	914	CLA	CMB-C2B-C3B	3.41	131.59	125.16
36	L	101	LHG	O4-P-O5	3.41	131.02	112.14
26	a	401	SQD	O5-C5-C6	3.41	113.19	105.91
23	c	906	CLA	C3B-CAB-CBB	-3.41	118.89	125.95
23	B	613	CLA	C4B-C3B-CAB	-3.41	120.27	127.18
23	c	904	CLA	OBD-CAD-C3D	-3.41	121.26	128.15
23	c	914	CLA	O2D-CGD-O1D	-3.41	116.95	123.79
23	B	605	CLA	CHD-C4C-C3C	-3.40	119.74	124.97
23	c	909	CLA	CHD-C4C-C3C	-3.41	119.74	124.97
23	C	509	CLA	CHC-C4B-NB	3.40	130.47	124.70
25	t	101	BCR	C35-C13-C12	3.40	123.58	118.09
23	b	614	CLA	O2D-CGD-O1D	-3.40	116.97	123.79
23	a	410	CLA	CHC-C4B-NB	3.39	130.46	124.70
23	C	504	CLA	O2D-CGD-CBD	3.39	118.19	111.34
23	b	619	CLA	CMD-C2D-C3D	3.39	131.55	125.16
23	c	910	CLA	C4B-NB-C1B	-3.39	103.85	107.12
23	B	611	CLA	C3A-C4A-CHB	-3.39	117.28	124.33
33	c	924	HTG	C2-C1-S1	-3.39	107.15	110.97
36	L	101	LHG	O7-C7-C8	3.39	118.76	111.54
23	b	612	CLA	C2D-C1D-ND	3.39	113.43	109.56
23	C	505	CLA	CAC-C3C-C4C	3.39	129.94	124.85
23	b	606	CLA	C3B-C4B-NB	3.39	113.59	109.21
25	B	618	BCR	C7-C8-C9	-3.39	121.15	126.22
23	a	410	CLA	C4B-C3B-CAB	-3.38	120.32	127.18
23	c	903	CLA	CMD-C2D-C3D	3.38	131.54	125.16
23	b	615	CLA	C4-C3-C5	3.38	120.53	115.39
23	A	410	CLA	C3B-C4B-NB	3.38	113.58	109.21
23	B	617	CLA	CBD-CHA-C1A	3.38	133.19	128.77
23	B	606	CLA	CHC-C4B-NB	3.38	130.44	124.70
23	C	505	CLA	C3B-CAB-CBB	-3.37	118.96	125.95
23	B	603	CLA	O2D-CGD-O1D	-3.37	117.02	123.79
23	b	619	CLA	CAC-C3C-C4C	3.37	129.91	124.85
23	C	505	CLA	CMC-C2C-C1C	3.37	129.76	124.95
23	b	614	CLA	CMC-C2C-C1C	3.37	129.76	124.95
23	B	613	CLA	C3B-C4B-CHC	-3.37	119.61	126.00
23	a	410	CLA	CGD-CBD-CHA	-3.37	105.84	113.65
33	B	625	HTG	C2-C1-S1	3.37	114.76	110.97
25	a	415	BCR	C38-C26-C25	-3.37	120.69	124.50
23	C	502	CLA	CMC-C2C-C1C	3.37	129.75	124.95
23	c	912	CLA	C3B-C2B-C1B	-3.36	102.96	106.69
28	a	419	PL9	C42-C43-C44	-3.36	120.54	127.81
23	c	905	CLA	CAC-C3C-C4C	3.36	129.90	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	414	PL9	C37-C38-C39	-3.36	120.55	127.81
23	B	615	CLA	CHC-C4B-NB	3.36	130.40	124.70
23	b	615	CLA	C3B-C2B-C1B	-3.36	102.97	106.69
23	c	905	CLA	O2D-CGD-CBD	3.36	118.12	111.34
28	a	419	PL9	C30-C29-C31	3.36	120.48	115.39
23	d	402	CLA	C3B-C2B-C1B	-3.35	102.97	106.69
30	B	623	LMT	O1'-C1'-C2'	3.35	112.45	108.15
23	B	610	CLA	CMB-C2B-C3B	3.35	131.48	125.16
23	c	909	CLA	C4A-NA-C1A	3.35	111.10	106.38
23	B	617	CLA	O2D-CGD-CBD	3.35	118.11	111.34
23	b	610	CLA	C3B-C4B-CHC	-3.35	119.65	126.00
23	c	913	CLA	CHD-C4C-C3C	-3.35	119.83	124.97
23	b	606	CLA	C4B-CHC-C1C	-3.34	123.07	127.47
23	C	508	CLA	C3B-C2B-C1B	-3.34	102.98	106.69
23	C	511	CLA	CMD-C2D-C3D	3.34	131.46	125.16
23	b	608	CLA	C3B-C4B-CHC	-3.34	119.66	126.00
23	b	607	CLA	C4A-NA-C1A	3.34	111.09	106.38
23	C	513	CLA	C4B-C3B-CAB	-3.34	120.42	127.18
23	C	505	CLA	C1C-C2C-C3C	-3.34	102.76	106.96
23	c	911	CLA	CMD-C2D-C3D	3.33	131.44	125.16
23	C	503	CLA	CHC-C4B-NB	3.33	130.36	124.70
23	c	904	CLA	C1C-C2C-C3C	-3.33	102.77	106.96
23	B	613	CLA	C2B-C3B-CAB	3.33	134.15	127.33
23	b	604	CLA	O2D-CGD-O1D	-3.33	117.10	123.79
23	B	609	CLA	C2A-C1A-NA	3.33	115.59	111.33
23	c	912	CLA	CMD-C2D-C3D	3.33	131.43	125.16
25	K	102	BCR	C20-C21-C22	-3.33	122.48	127.29
23	b	608	CLA	CGD-CBD-CHA	-3.33	105.94	113.65
24	a	412	PHO	C1C-C2C-C3C	-3.33	102.47	106.55
23	B	613	CLA	CMD-C2D-C3D	3.33	131.44	125.16
23	a	409	CLA	C1C-C2C-C3C	-3.33	102.78	106.96
34	C	517	DGD	CGB-CFB-CEB	-3.33	103.43	112.94
23	B	605	CLA	C4-C3-C5	3.33	120.44	115.39
28	a	419	PL9	C35-C34-C36	3.32	120.44	115.39
23	b	605	CLA	C4-C3-C5	3.32	120.43	115.39
26	A	418	SQD	C1-O5-C5	-3.32	107.31	113.73
23	b	616	CLA	C3C-C4C-NC	3.32	114.15	110.15
23	b	613	CLA	C4D-ND-C1D	-3.32	102.56	106.57
24	A	408	PHO	C4C-NC-C1C	-3.32	99.91	106.52
25	A	411	BCR	C11-C10-C9	-3.32	122.50	127.29
23	B	607	CLA	C4-C3-C5	3.32	120.43	115.39
23	c	914	CLA	C1C-C2C-C3C	-3.32	102.79	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C2B-C1B-CHB	-3.31	119.72	126.00
23	D	402	CLA	CHC-C1C-C2C	-3.31	117.61	126.51
23	B	605	CLA	O2D-CGD-O1D	-3.31	117.13	123.79
23	a	411	CLA	CBA-CAA-C2A	-3.31	105.85	113.95
23	a	411	CLA	C2A-C1A-CHA	-3.31	117.85	123.87
23	c	912	CLA	C4B-C3B-C2B	-3.31	103.64	107.04
23	B	604	CLA	C3B-CAB-CBB	-3.31	119.10	125.95
23	c	910	CLA	C1C-C2C-C3C	-3.31	102.80	106.96
23	A	410	CLA	C4B-NB-C1B	-3.31	103.94	107.12
23	C	507	CLA	CMB-C2B-C3B	3.31	131.39	125.16
23	b	609	CLA	C1C-C2C-C3C	-3.31	102.80	106.96
23	b	611	CLA	C3C-C4C-NC	3.30	114.13	110.15
33	V	202	HTG	O5-C5-C6	3.30	114.57	106.34
23	B	605	CLA	C2D-C1D-ND	3.30	113.33	109.56
23	b	614	CLA	CBC-CAC-C3C	-3.30	102.37	112.37
23	A	406	CLA	CBD-CHA-C1A	3.30	133.08	128.77
23	b	614	CLA	O2D-CGD-CBD	3.30	118.01	111.34
23	C	501	CLA	CAC-C3C-C4C	3.30	129.80	124.85
23	A	407	CLA	CHD-C4C-C3C	-3.30	119.91	124.97
23	c	910	CLA	CGD-CBD-CHA	-3.30	106.00	113.65
23	C	512	CLA	CBA-CAA-C2A	-3.30	105.89	113.95
23	B	608	CLA	C1C-C2C-C3C	-3.29	102.82	106.96
23	b	610	CLA	C2D-C1D-ND	3.29	113.32	109.56
23	b	617	CLA	C3B-C4B-NB	3.29	113.46	109.21
23	C	513	CLA	C4A-NA-C1A	3.29	111.01	106.38
23	b	605	CLA	C1-C2-C3	-3.29	120.53	126.23
26	a	416	SQD	C45-O47-C7	-3.29	110.13	117.86
25	b	621	BCR	C29-C30-C25	3.29	115.61	110.37
34	C	517	DGD	O2G-C1B-O1B	-3.29	114.89	123.66
23	b	606	CLA	O2A-C1-C2	-3.29	100.59	108.12
30	a	402	LMT	O5'-C1'-O1'	-3.28	102.11	109.93
23	c	903	CLA	C3B-C4B-CHC	-3.28	119.77	126.00
23	B	611	CLA	O2A-CGA-CBA	3.28	121.95	111.90
23	B	611	CLA	C4D-ND-C1D	-3.28	102.60	106.57
23	d	402	CLA	C3C-C4C-NC	3.28	114.11	110.15
23	a	410	CLA	C3A-C4A-NA	3.28	114.78	110.81
23	c	908	CLA	C3C-C4C-NC	3.28	114.10	110.15
34	h	102	DGD	O1G-C1A-C2A	3.28	121.93	111.90
26	D	407	SQD	O48-C23-C24	3.27	121.92	111.90
23	B	614	CLA	C2B-C3B-CAB	3.27	134.02	127.33
23	b	607	CLA	C3B-C2B-C1B	-3.27	103.07	106.69
25	C	514	BCR	C7-C8-C9	-3.27	121.33	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C5-C3-C2	-3.27	114.78	121.06
34	h	102	DGD	O1G-C1A-O1A	-3.27	114.94	123.48
23	b	612	CLA	C2A-C1A-NA	3.27	115.51	111.33
23	B	612	CLA	CBD-CHA-C1A	3.27	133.04	128.77
23	b	619	CLA	C3B-C4B-CHC	-3.27	119.81	126.00
23	b	619	CLA	C3B-CAB-CBB	-3.27	119.19	125.95
25	c	916	BCR	C38-C26-C25	-3.26	120.81	124.50
34	c	917	DGD	O5D-C6D-C5D	-3.26	103.31	108.96
23	C	513	CLA	CMD-C2D-C3D	3.26	131.30	125.16
24	a	413	PHO	C1D-CHD-C4C	-3.26	119.98	126.23
23	B	611	CLA	C3B-C2B-C1B	-3.26	103.08	106.69
23	B	611	CLA	C3B-C4B-NB	3.26	113.42	109.21
26	D	407	SQD	O9-S-O7	-3.26	102.13	113.45
34	c	919	DGD	O1G-C1A-C2A	3.26	121.86	111.90
28	a	419	PL9	C40-C39-C41	3.25	120.33	115.39
25	B	619	BCR	C29-C30-C25	3.25	115.56	110.37
23	D	402	CLA	C3A-C4A-NA	3.25	114.74	110.81
23	C	503	CLA	CBD-CHA-C1A	3.25	133.02	128.77
23	c	902	CLA	CMD-C2D-C1D	3.25	132.59	126.16
23	c	907	CLA	C1-C2-C3	-3.25	120.58	126.23
23	c	911	CLA	C3B-C2B-C1B	-3.25	103.09	106.69
23	B	613	CLA	C3C-C4C-NC	3.25	114.07	110.15
34	d	406	DGD	O6D-C1D-O3G	3.25	117.67	109.93
25	t	101	BCR	C12-C13-C14	-3.25	113.98	118.98
23	B	611	CLA	C4B-NB-C1B	-3.25	103.99	107.12
23	C	511	CLA	C1-O2A-CGA	3.25	126.44	117.00
23	d	402	CLA	C2D-C1D-ND	3.24	113.26	109.56
23	b	618	CLA	CAC-C3C-C4C	3.24	129.72	124.85
28	a	419	PL9	C7-C3-C2	-3.24	120.80	123.75
23	A	406	CLA	C3C-C4C-NC	3.24	114.05	110.15
25	K	102	BCR	C38-C26-C25	-3.24	120.84	124.50
38	H	101	RRX	C16-C15-C14	-3.23	116.33	123.45
23	B	609	CLA	O2A-CGA-CBA	3.23	121.79	111.90
23	A	406	CLA	C2D-C1D-ND	3.23	113.24	109.56
24	A	409	PHO	CBA-CAA-C2A	-3.23	106.06	113.95
23	A	406	CLA	C2B-C3B-CAB	3.22	133.92	127.33
23	B	613	CLA	C4-C3-C5	3.22	120.29	115.39
23	B	616	CLA	C1D-CHD-C4C	-3.22	117.60	122.60
23	C	506	CLA	C4B-NB-C1B	3.22	110.22	107.12
25	A	411	BCR	C15-C16-C17	-3.22	116.35	123.45
34	c	919	DGD	O3G-C3G-C2G	-3.22	103.34	110.99
25	B	618	BCR	C24-C23-C22	-3.21	121.41	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	909	CLA	C4B-C3B-C2B	-3.21	103.74	107.04
23	B	608	CLA	CED-O2D-CGD	3.21	123.65	116.00
25	A	411	BCR	C8-C7-C6	-3.21	117.75	127.23
27	A	413	LMG	O6-C1-C2	-3.21	103.73	110.30
25	T	101	BCR	C7-C8-C9	-3.21	121.42	126.22
23	c	913	CLA	C1C-C2C-C3C	-3.21	102.92	106.96
23	b	605	CLA	CMB-C2B-C1B	-3.21	123.54	128.46
23	B	610	CLA	O2D-CGD-CBD	3.21	117.82	111.34
24	a	413	PHO	C3C-C4C-NC	3.20	114.81	109.87
23	D	403	CLA	CHD-C4C-C3C	-3.20	120.05	124.97
23	B	607	CLA	C4A-NA-C1A	3.20	110.90	106.38
23	B	614	CLA	C1-C2-C3	-3.20	120.67	126.23
23	c	906	CLA	C4B-C3B-CAB	-3.20	120.70	127.18
23	b	609	CLA	O2D-CGD-O1D	-3.20	117.37	123.79
23	B	615	CLA	CBC-CAC-C3C	-3.20	102.69	112.37
23	C	501	CLA	C2A-C1A-CHA	-3.20	118.05	123.87
25	t	101	BCR	C33-C5-C6	-3.19	120.89	124.50
23	b	614	CLA	C4B-CHC-C1C	-3.19	123.27	127.47
23	C	512	CLA	C3B-C4B-CHC	-3.19	119.95	126.00
26	A	418	SQD	C1-C2-C3	-3.19	103.81	109.99
23	c	911	CLA	O2D-CGD-CBD	3.19	117.78	111.34
23	a	410	CLA	C1C-C2C-C3C	-3.19	102.95	106.96
23	a	414	CLA	C3B-C2B-C1B	-3.19	103.16	106.69
23	c	905	CLA	C3B-C2B-C1B	-3.19	103.16	106.69
27	Z	101	LMG	C3-C4-C5	3.18	115.88	110.17
23	b	613	CLA	O2D-CGD-CBD	3.18	117.77	111.34
23	b	617	CLA	CHB-C4A-NA	3.18	128.82	124.38
25	K	102	BCR	C33-C5-C6	-3.18	120.91	124.50
23	C	507	CLA	C3B-C4B-CHC	-3.18	119.97	126.00
23	C	510	CLA	O2D-CGD-O1D	-3.18	117.41	123.79
23	B	607	CLA	O2D-CGD-CBD	3.18	117.76	111.34
23	a	411	CLA	C3B-C2B-C1B	-3.17	103.17	106.69
23	B	607	CLA	C2B-C3B-CAB	3.17	133.82	127.33
23	A	410	CLA	CGD-CBD-CHA	-3.17	106.30	113.65
23	A	405	CLA	CAA-CBA-CGA	-3.17	103.91	113.24
30	C	520	LMT	O3'-C3'-C4'	3.17	117.28	109.86
23	c	914	CLA	O2A-CGA-CBA	3.16	121.58	111.90
23	b	608	CLA	CMD-C2D-C1D	3.16	132.41	126.16
23	B	607	CLA	C3B-C4B-NB	3.16	113.30	109.21
27	C	519	LMG	O5-C6-C5	-3.15	100.38	111.37
23	B	616	CLA	C4-C3-C5	3.15	120.18	115.39
23	B	614	CLA	CHC-C4B-NB	3.15	130.06	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	405	PL9	C36-C37-C38	-3.15	102.68	111.64
24	A	409	PHO	O2D-CGD-O1D	-3.15	117.46	123.79
23	D	403	CLA	CAC-C3C-C4C	3.15	129.58	124.85
23	C	509	CLA	O2A-CGA-CBA	3.15	121.53	111.90
23	D	402	CLA	C1D-CHD-C4C	-3.14	117.73	122.60
23	C	503	CLA	O2D-CGD-CBD	3.14	117.68	111.34
23	c	914	CLA	C2D-C1D-ND	3.14	113.14	109.56
23	a	410	CLA	CBC-CAC-C3C	-3.14	102.87	112.37
23	C	505	CLA	C4B-C3B-CAB	-3.14	120.83	127.18
23	C	508	CLA	C3B-C4B-CHC	-3.13	120.06	126.00
23	A	405	CLA	C4B-C3B-C2B	-3.13	103.82	107.04
28	A	414	PL9	C30-C29-C31	3.13	120.15	115.39
25	t	101	BCR	C1-C6-C7	3.13	124.38	115.69
23	B	613	CLA	O2D-CGD-O1D	-3.13	117.50	123.79
23	D	403	CLA	C4D-ND-C1D	-3.13	102.79	106.57
23	A	406	CLA	C1D-CHD-C4C	-3.13	117.75	122.60
23	B	603	CLA	C2B-C3B-CAB	3.13	133.72	127.33
34	C	518	DGD	O1G-C1A-C2A	3.12	121.46	111.90
23	B	613	CLA	O2D-CGD-CBD	3.12	117.65	111.34
25	a	415	BCR	C7-C8-C9	-3.12	121.54	126.22
23	C	513	CLA	C4-C3-C5	3.12	120.13	115.39
26	f	102	SQD	O48-C23-C24	3.12	121.46	111.90
27	B	622	LMG	C31-C30-C29	-3.12	101.72	113.28
25	K	102	BCR	C16-C17-C18	-3.11	122.79	127.29
23	c	911	CLA	C1C-C2C-C3C	-3.11	103.04	106.96
23	b	615	CLA	CMD-C2D-C3D	3.11	131.03	125.16
23	c	912	CLA	C3B-C4B-CHC	-3.11	120.10	126.00
23	c	907	CLA	C1C-C2C-C3C	-3.11	103.05	106.96
28	A	414	PL9	C3-C4-C5	3.11	123.02	118.69
23	D	403	CLA	C4B-C3B-CAB	-3.11	120.88	127.18
23	c	910	CLA	C4D-C3D-CAD	3.11	111.87	108.05
28	D	405	PL9	C22-C23-C24	-3.11	121.09	127.81
23	A	405	CLA	C3B-C4B-CHC	-3.11	120.11	126.00
23	a	414	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
23	c	906	CLA	CMD-C2D-C3D	3.10	131.01	125.16
23	c	914	CLA	O2D-CGD-CBD	3.10	117.60	111.34
23	B	604	CLA	O2A-CGA-O1A	-3.10	115.38	123.48
24	a	412	PHO	C3B-CAB-CBB	-3.10	119.53	125.95
23	D	403	CLA	C2B-C3B-CAB	3.10	133.66	127.33
27	C	519	LMG	O8-C28-O10	-3.10	115.38	123.48
23	b	608	CLA	C3B-C2B-C1B	-3.10	103.26	106.69
23	C	502	CLA	C4-C3-C5	3.09	120.09	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CMC-C2C-C1C	3.09	129.35	124.95
36	d	408	LHG	C34-C33-C32	-3.09	98.17	114.56
27	c	920	LMG	O5-C6-C5	-3.09	100.62	111.37
30	a	402	LMT	O2'-C2'-C1'	3.08	116.74	110.03
23	b	617	CLA	C4B-C3B-C2B	-3.08	103.88	107.04
23	b	613	CLA	CAA-CBA-CGA	-3.08	104.16	113.24
25	k	101	BCR	C38-C26-C25	-3.08	121.02	124.50
23	b	610	CLA	C4B-C3B-C2B	-3.08	103.87	107.04
23	c	902	CLA	C4B-C3B-CAB	-3.08	120.94	127.18
25	b	620	BCR	C35-C13-C12	3.08	123.06	118.09
25	b	620	BCR	C24-C23-C22	-3.08	121.61	126.22
23	C	512	CLA	C1C-C2C-C3C	-3.08	103.09	106.96
23	a	414	CLA	C1C-NC-C4C	-3.08	102.11	106.26
23	d	402	CLA	C5-C3-C2	-3.08	115.15	121.06
23	B	603	CLA	C3B-C2B-C1B	-3.08	103.28	106.69
23	a	411	CLA	O2D-CGD-CBD	3.08	117.56	111.34
23	B	602	CLA	O1D-CGD-CBD	-3.07	118.17	124.45
23	c	907	CLA	C4D-ND-C1D	-3.07	102.85	106.57
33	c	924	HTG	C3-C4-C5	3.07	115.69	110.17
23	B	617	CLA	C1-O2A-CGA	3.07	125.93	117.00
23	B	614	CLA	C3B-CAB-CBB	-3.07	119.59	125.95
23	b	608	CLA	C3A-C2A-C1A	-3.07	96.72	101.70
23	C	509	CLA	C1-C2-C3	-3.07	120.91	126.23
23	b	613	CLA	CHB-C4A-NA	3.07	128.66	124.38
23	C	504	CLA	CAC-C3C-C4C	3.06	129.45	124.85
23	A	407	CLA	CHD-C4C-NC	3.06	126.42	124.28
23	c	910	CLA	C1-C2-C3	-3.06	120.92	126.23
23	C	502	CLA	O2D-CGD-O1D	-3.06	117.65	123.79
23	B	616	CLA	C4A-NA-C1A	3.06	110.69	106.38
30	M	102	LMT	C3'-C4'-C5'	-3.05	104.03	110.86
36	D	410	LHG	O4-P-O5	3.05	129.05	112.14
23	a	414	CLA	C3A-C4A-NA	3.05	114.50	110.81
34	d	406	DGD	O1G-C1G-C2G	3.05	116.83	108.80
23	c	906	CLA	C2B-C3B-CAB	3.05	133.57	127.33
30	C	520	LMT	C1B-O5B-C5B	3.05	119.64	113.73
23	b	611	CLA	O2A-CGA-O1A	-3.05	115.50	123.48
25	T	101	BCR	C15-C16-C17	-3.05	116.73	123.45
28	d	405	PL9	C31-C32-C33	-3.05	102.97	111.64
34	c	918	DGD	O6E-C5E-C4E	-3.05	104.07	109.73
28	D	405	PL9	C53-C6-C1	3.05	122.22	114.99
23	A	410	CLA	CAC-C3C-C4C	3.05	129.43	124.85
23	C	506	CLA	CAC-C3C-C4C	3.05	129.42	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	908	CLA	CHC-C4B-NB	3.05	129.88	124.70
23	C	501	CLA	C3C-C4C-NC	3.05	113.82	110.15
23	C	511	CLA	C4B-CHC-C1C	-3.05	123.46	127.47
23	b	613	CLA	C4A-NA-C1A	3.05	110.67	106.38
24	a	413	PHO	C1-C2-C3	-3.05	120.94	126.23
23	B	610	CLA	CBC-CAC-C3C	-3.05	103.15	112.37
23	B	606	CLA	C2A-C1A-CHA	-3.04	118.33	123.87
23	C	508	CLA	CHD-C4C-C3C	-3.04	120.30	124.97
34	C	516	DGD	C3G-C2G-C1G	-3.04	104.88	111.86
23	A	406	CLA	OBD-CAD-C3D	-3.04	122.01	128.15
23	c	914	CLA	C3B-C4B-CHC	-3.04	120.24	126.00
23	A	406	CLA	CBC-CAC-C3C	-3.04	103.17	112.37
25	T	101	BCR	C2-C1-C6	3.04	115.21	110.37
23	B	602	CLA	CMD-C2D-C1D	3.04	132.16	126.16
23	B	613	CLA	C3B-CAB-CBB	-3.04	119.66	125.95
23	b	606	CLA	C4B-C3B-CAB	-3.04	121.03	127.18
23	C	513	CLA	CHC-C4B-NB	3.03	129.85	124.70
24	A	408	PHO	C4B-C3B-C2B	-3.03	104.78	106.90
23	c	910	CLA	O2D-CGD-CBD	3.03	117.47	111.34
24	A	408	PHO	CBA-CAA-C2A	-3.03	106.53	113.95
34	c	918	DGD	C3E-C4E-C5E	3.03	115.61	110.17
23	b	617	CLA	C4-C3-C5	3.03	119.99	115.39
23	b	606	CLA	CAC-C3C-C4C	3.03	129.40	124.85
23	d	403	CLA	C2A-C1A-NA	3.03	115.21	111.33
24	A	409	PHO	CAA-C2A-C1A	-3.03	104.76	112.78
23	B	611	CLA	CGD-CBD-CHA	-3.03	106.63	113.65
26	B	621	SQD	C4-C3-C2	3.03	116.38	110.80
25	k	101	BCR	C24-C23-C22	-3.03	121.69	126.22
23	B	613	CLA	C4B-NB-C1B	3.03	110.03	107.12
25	a	415	BCR	C16-C15-C14	-3.02	116.79	123.45
23	b	612	CLA	C4C-C3C-C2C	-3.02	101.97	106.93
23	B	612	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
23	b	609	CLA	CMC-C2C-C3C	3.02	134.67	126.04
23	C	512	CLA	CMD-C2D-C3D	3.02	130.86	125.16
23	B	617	CLA	C2A-C1A-NA	3.02	115.20	111.33
23	a	409	CLA	C7-C6-C5	-3.02	104.15	112.97
31	C	524	GOL	O3-C3-C2	-3.02	96.94	110.37
23	C	506	CLA	C4-C3-C5	3.02	119.97	115.39
23	c	909	CLA	C3B-C4B-NB	3.02	113.11	109.21
23	c	905	CLA	C4A-NA-C1A	3.02	110.64	106.38
23	c	914	CLA	CMD-C2D-C3D	3.02	130.85	125.16
23	b	615	CLA	C3B-C4B-NB	3.02	113.11	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	CHC-C4B-NB	3.02	129.82	124.70
23	C	509	CLA	C2D-C1D-ND	3.01	113.00	109.56
23	B	614	CLA	C2A-C1A-CHA	-3.02	118.38	123.87
23	b	606	CLA	CHC-C4B-NB	3.01	129.82	124.70
23	b	609	CLA	O2D-CGD-CBD	3.01	117.43	111.34
23	B	606	CLA	C4B-CHC-C1C	-3.01	123.51	127.47
23	c	907	CLA	O2A-CGA-O1A	-3.01	115.61	123.48
33	b	626	HTG	C1-O5-C5	3.01	118.73	112.78
23	b	617	CLA	C1C-C2C-C3C	-3.01	103.18	106.96
23	B	604	CLA	C2A-C1A-CHA	-3.00	118.41	123.87
23	B	604	CLA	CMB-C2B-C3B	3.00	130.82	125.16
23	b	616	CLA	C3B-C4B-NB	3.00	113.09	109.21
30	M	101	LMT	C1-O1'-C1'	3.00	119.21	113.91
23	B	611	CLA	C1C-C2C-C3C	-3.00	103.18	106.96
25	C	514	BCR	C11-C10-C9	-3.00	122.95	127.29
34	C	516	DGD	O1G-C1G-C2G	-3.00	100.91	108.80
23	c	913	CLA	O2D-CGD-O1D	-3.00	117.77	123.79
23	C	508	CLA	C4B-C3B-C2B	-3.00	103.96	107.04
23	A	410	CLA	CHC-C4B-NB	3.00	129.79	124.70
23	b	611	CLA	C3B-C4B-NB	2.99	113.08	109.21
23	c	909	CLA	C3B-C4B-CHC	-2.99	120.33	126.00
23	B	605	CLA	CHC-C4B-NB	2.99	129.78	124.70
25	t	101	BCR	C7-C6-C5	-2.99	114.39	121.59
23	D	402	CLA	CMB-C2B-C3B	2.98	130.78	125.16
23	c	903	CLA	C3B-C4B-NB	2.98	113.07	109.21
23	C	508	CLA	C2D-C3D-CAD	2.98	147.09	134.94
36	D	408	LHG	O4-P-O5	2.98	128.63	112.14
23	C	506	CLA	O2D-CGD-O1D	-2.98	117.81	123.79
36	E	101	LHG	O3-C3-C2	2.98	118.15	108.54
25	T	101	BCR	C12-C13-C14	-2.97	114.40	118.98
24	a	412	PHO	C4C-NC-C1C	-2.97	100.60	106.52
24	A	409	PHO	C4B-NB-C1B	-2.97	102.92	108.29
24	A	409	PHO	C2B-C1B-NB	2.97	116.68	106.15
23	B	603	CLA	CBD-CHA-C1A	2.97	132.65	128.77
34	c	917	DGD	C6D-O5D-C1E	-2.97	107.84	113.80
23	a	411	CLA	C3B-C4B-NB	2.97	113.05	109.21
23	b	609	CLA	C3B-C4B-NB	2.97	113.05	109.21
23	C	504	CLA	CHD-C4C-C3C	-2.97	120.41	124.97
23	d	403	CLA	C4B-C3B-C2B	-2.97	103.99	107.04
25	d	404	BCR	C40-C30-C25	-2.97	105.42	110.33
23	b	612	CLA	O2D-CGD-O1D	-2.97	117.83	123.79
23	c	911	CLA	C4-C3-C2	-2.97	117.62	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	PHO	CMB-C2B-C3B	2.96	130.75	125.16
23	C	509	CLA	O2A-CGA-O1A	-2.96	115.73	123.48
23	B	614	CLA	C4B-C3B-CAB	-2.97	121.17	127.18
23	D	403	CLA	CMA-C3A-C4A	-2.96	102.93	112.40
38	h	101	RRX	C16-C17-C18	-2.96	123.01	127.29
23	B	610	CLA	C1C-C2C-C3C	-2.96	103.24	106.96
23	a	411	CLA	C2D-C1D-ND	2.96	112.94	109.56
25	b	621	BCR	C16-C17-C18	2.96	131.57	127.29
23	c	907	CLA	C3B-C4B-NB	2.96	113.03	109.21
23	b	618	CLA	C3B-C4B-NB	2.96	113.03	109.21
23	B	603	CLA	O2D-CGD-CBD	2.95	117.31	111.34
23	c	913	CLA	C3B-C4B-CHC	-2.95	120.40	126.00
23	a	414	CLA	CMB-C2B-C3B	2.95	130.72	125.16
23	b	606	CLA	C4B-C3B-C2B	-2.95	104.01	107.04
23	b	616	CLA	O2D-CGD-O1D	-2.95	117.87	123.79
23	C	509	CLA	CMC-C2C-C3C	2.95	134.45	126.04
23	D	402	CLA	CBD-CHA-C1A	2.95	132.62	128.77
28	a	419	PL9	C45-C44-C46	2.95	119.87	115.39
24	a	412	PHO	C2C-C1C-NC	2.95	117.36	110.51
23	b	619	CLA	C4C-C3C-C2C	-2.95	102.10	106.93
36	d	409	LHG	O4-P-O5	2.94	128.41	112.14
23	A	410	CLA	C2B-C3B-CAB	2.94	133.34	127.33
23	c	909	CLA	C1C-C2C-C3C	-2.94	103.27	106.96
23	C	509	CLA	C3B-CAB-CBB	-2.94	119.87	125.95
23	B	603	CLA	C3B-CAB-CBB	-2.94	119.87	125.95
25	A	411	BCR	C7-C8-C9	-2.94	121.82	126.22
23	B	612	CLA	C2A-C1A-NA	2.94	115.09	111.33
23	b	617	CLA	C4A-NA-C1A	2.93	110.52	106.38
24	A	408	PHO	C2C-C1C-NC	2.93	117.33	110.51
30	A	419	LMT	O1'-C1'-C2'	2.93	111.91	108.15
23	b	612	CLA	C2D-C3D-CAD	2.93	146.90	134.94
23	a	409	CLA	CMD-C2D-C3D	2.93	130.69	125.16
23	B	611	CLA	C3B-C4B-CHC	-2.93	120.44	126.00
23	C	501	CLA	CBC-CAC-C3C	-2.93	103.49	112.37
23	C	505	CLA	O2D-CGD-CBD	2.93	117.26	111.34
34	C	517	DGD	O2G-C1B-C2B	2.93	117.78	111.54
23	B	613	CLA	CHD-C4C-NC	2.93	126.33	124.28
23	C	509	CLA	CMB-C2B-C1B	2.93	132.97	128.46
23	b	605	CLA	C2A-C3A-C4A	-2.93	97.16	101.89
23	c	909	CLA	C1-C2-C3	-2.93	121.15	126.23
23	B	609	CLA	C2A-C1A-CHA	-2.93	118.55	123.87
23	B	605	CLA	CGD-CBD-CAD	-2.92	100.97	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C3C-C4C-NC	2.93	113.68	110.15
23	B	607	CLA	C3C-C4C-NC	2.93	113.68	110.15
23	B	606	CLA	O2D-CGD-CBD	2.92	117.24	111.34
24	a	412	PHO	CMC-C2C-C1C	2.92	129.87	125.03
24	a	412	PHO	CAC-C3C-C4C	2.92	128.71	125.18
23	b	612	CLA	CGD-CBD-CHA	-2.92	106.88	113.65
23	B	607	CLA	CHC-C4B-NB	2.92	129.66	124.70
25	C	515	BCR	C33-C5-C6	-2.92	121.20	124.50
23	C	501	CLA	O1D-CGD-CBD	-2.92	118.50	124.45
23	B	614	CLA	C4B-CHC-C1C	-2.92	123.64	127.47
23	a	409	CLA	CAC-C3C-C2C	-2.91	122.25	127.50
23	a	414	CLA	C2B-C3B-CAB	2.91	133.28	127.33
25	D	404	BCR	C10-C11-C12	-2.91	113.45	123.23
23	b	604	CLA	C1-O2A-CGA	2.91	125.47	117.00
23	c	906	CLA	CMC-C2C-C1C	2.91	129.10	124.95
37	F	101	HEM	CMA-C3A-C4A	-2.91	123.99	128.46
23	C	510	CLA	C4-C3-C5	2.91	119.81	115.39
23	C	509	CLA	O2D-CGD-CBD	2.91	117.22	111.34
30	M	101	LMT	O2'-C2'-C1'	2.91	116.35	110.03
33	B	624	HTG	C3'-C2'-C1'	-2.90	101.08	113.28
25	t	101	BCR	C20-C21-C22	-2.90	123.09	127.29
23	b	610	CLA	C2B-C3B-CAB	2.90	133.27	127.33
23	B	612	CLA	C2B-C1B-CHB	-2.90	120.50	126.00
23	A	406	CLA	C1C-NC-C4C	-2.90	102.35	106.26
23	B	609	CLA	C3A-C4A-NA	2.90	114.32	110.81
23	C	507	CLA	O2D-CGD-CBD	2.90	117.20	111.34
25	b	621	BCR	C8-C7-C6	-2.90	118.68	127.23
23	d	402	CLA	C3A-C4A-CHB	-2.90	118.31	124.33
36	L	101	LHG	O6-P-O3	-2.89	96.42	104.68
28	A	414	PL9	C45-C44-C46	2.89	119.78	115.39
23	D	403	CLA	C3B-C4B-NB	2.89	112.95	109.21
23	C	508	CLA	O2A-CGA-O1A	-2.89	115.93	123.48
23	b	608	CLA	CHD-C4C-NC	2.89	126.30	124.28
23	c	909	CLA	CMA-C3A-C4A	-2.89	103.16	112.40
23	c	908	CLA	CMD-C2D-C3D	2.89	130.60	125.16
23	b	608	CLA	CHC-C4B-NB	2.89	129.60	124.70
23	C	503	CLA	C4-C3-C5	2.89	119.77	115.39
25	B	618	BCR	C16-C15-C14	-2.88	117.10	123.45
23	C	506	CLA	C1-C2-C3	-2.88	121.23	126.23
23	C	503	CLA	C3C-C4C-NC	2.88	113.63	110.15
23	B	604	CLA	C1D-CHD-C4C	-2.88	118.13	122.60
23	a	410	CLA	C3C-C4C-NC	2.88	113.63	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	CMC-C2C-C1C	2.88	129.06	124.95
23	C	509	CLA	O2D-CGD-O1D	-2.88	118.00	123.79
23	B	614	CLA	C1C-C2C-C3C	-2.88	103.33	106.96
30	B	623	LMT	O5B-C5B-C4B	2.88	115.09	109.73
23	B	612	CLA	C4B-NB-C1B	-2.88	104.34	107.12
23	B	603	CLA	C1-C2-C3	-2.88	121.23	126.23
23	b	609	CLA	O2A-CGA-O1A	-2.88	115.95	123.48
23	a	411	CLA	C1-C2-C3	-2.88	121.23	126.23
34	c	918	DGD	O5D-C6D-C5D	2.88	113.95	108.96
23	C	506	CLA	CMD-C2D-C3D	2.88	130.58	125.16
37	f	101	HEM	CMC-C2C-C3C	2.88	131.06	124.26
23	A	410	CLA	O2D-CGD-CBD	2.88	117.15	111.34
26	f	102	SQD	C46-O48-C23	2.88	125.20	116.99
23	b	610	CLA	C3B-C2B-C1B	-2.87	103.50	106.69
34	c	919	DGD	O1G-C1A-O1A	-2.87	115.98	123.48
23	B	615	CLA	C4-C3-C2	-2.87	117.81	123.52
23	B	610	CLA	C2A-C1A-NA	2.87	115.00	111.33
23	B	606	CLA	O2A-C1-C2	-2.87	101.55	108.12
26	a	416	SQD	O5-C1-C2	-2.87	104.44	110.30
23	b	611	CLA	CMB-C2B-C3B	2.87	130.56	125.16
23	c	903	CLA	C1C-C2C-C3C	-2.87	103.36	106.96
23	b	617	CLA	C3B-C2B-C1B	-2.86	103.52	106.69
23	C	502	CLA	C1C-C2C-C3C	-2.86	103.36	106.96
26	D	407	SQD	C46-C45-C44	-2.86	105.28	111.86
23	b	611	CLA	CMD-C2D-C3D	2.86	130.56	125.16
23	D	402	CLA	CAA-CBA-CGA	-2.86	104.81	113.24
23	B	606	CLA	CAC-C3C-C4C	2.86	129.14	124.85
25	K	101	BCR	C40-C30-C25	-2.86	105.60	110.33
23	b	608	CLA	C1C-NC-C4C	-2.86	102.41	106.26
23	b	616	CLA	C3B-CAB-CBB	-2.86	120.03	125.95
23	c	910	CLA	CHB-C4A-NA	2.86	128.37	124.38
25	B	618	BCR	C10-C11-C12	-2.86	113.64	123.23
28	a	419	PL9	C15-C14-C16	2.86	119.73	115.39
23	C	505	CLA	C3C-C4C-NC	2.86	113.59	110.15
36	a	417	LHG	O8-C23-C24	2.86	120.64	111.90
23	B	614	CLA	C3B-C2B-C1B	-2.86	103.52	106.69
25	A	411	BCR	C28-C27-C26	-2.86	109.12	113.81
23	B	604	CLA	C4B-C3B-C2B	-2.85	104.11	107.04
23	A	407	CLA	C3C-C4C-NC	2.85	113.59	110.15
33	b	626	HTG	C1-C2-C3	2.85	116.68	110.72
34	c	918	DGD	O2G-C1B-C2B	2.85	117.61	111.54
23	B	615	CLA	O2A-CGA-O1A	-2.85	116.03	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C2A-C1A-CHA	-2.85	118.69	123.87
25	B	620	BCR	C7-C8-C9	-2.85	121.95	126.22
23	b	607	CLA	CHC-C4B-NB	2.85	129.53	124.70
26	B	621	SQD	O48-C23-O10	-2.85	116.04	123.48
23	B	613	CLA	O2A-C1-C2	-2.84	101.61	108.12
27	d	410	LMG	O8-C28-O10	-2.84	116.05	123.48
34	c	919	DGD	C3E-C4E-C5E	-2.84	105.08	110.17
23	B	605	CLA	C3B-CAB-CBB	-2.84	120.07	125.95
27	B	622	LMG	O5-C6-C5	-2.84	101.49	111.37
28	A	414	PL9	C53-C6-C1	2.83	121.71	114.99
23	C	503	CLA	O2D-CGD-O1D	-2.83	118.10	123.79
23	a	411	CLA	CBC-CAC-C3C	-2.83	103.80	112.37
23	b	611	CLA	C2B-C3B-CAB	2.83	133.12	127.33
36	d	408	LHG	O8-C23-O10	-2.83	116.08	123.48
23	B	615	CLA	C4B-C3B-C2B	-2.83	104.13	107.04
23	C	504	CLA	CMB-C2B-C3B	2.83	130.49	125.16
23	D	402	CLA	O2A-CGA-O1A	-2.83	116.09	123.48
23	A	406	CLA	CAC-C3C-C2C	-2.82	122.41	127.50
23	b	619	CLA	CGD-CBD-CHA	-2.82	107.10	113.65
23	b	616	CLA	C2B-C3B-CAB	2.82	133.10	127.33
36	l	101	LHG	O7-C7-O9	-2.82	116.12	123.66
23	B	607	CLA	C1-C2-C3	-2.82	121.33	126.23
23	B	606	CLA	C1C-C2C-C3C	-2.82	103.41	106.96
23	a	411	CLA	C3B-CAB-CBB	-2.82	120.11	125.95
23	b	616	CLA	C1C-C2C-C3C	-2.82	103.41	106.96
23	b	615	CLA	CGD-CBD-CHA	-2.82	107.11	113.65
37	V	201	HEM	CAD-CBD-CGD	-2.82	108.21	113.53
23	B	603	CLA	C4B-C3B-C2B	-2.82	104.14	107.04
23	D	402	CLA	C4-C3-C5	2.82	119.67	115.39
23	A	410	CLA	C5-C3-C2	-2.82	115.64	121.06
23	b	607	CLA	O2A-CGA-O1A	-2.82	116.11	123.48
34	H	102	DGD	C6D-C5D-C4D	2.82	118.37	111.98
26	L	103	SQD	O5-C1-C2	-2.81	104.54	110.30
23	C	504	CLA	C3B-C2B-C1B	-2.81	103.57	106.69
27	B	622	LMG	O8-C28-O10	-2.81	116.13	123.48
37	f	101	HEM	CMA-C3A-C4A	-2.81	124.15	128.46
23	c	908	CLA	C4A-NA-C1A	2.81	110.34	106.38
23	c	902	CLA	C4-C3-C5	2.81	119.66	115.39
30	m	101	LMT	O4'-C4B-C3B	2.81	116.62	110.36
23	c	909	CLA	C4D-ND-C1D	-2.81	103.18	106.57
23	A	406	CLA	C4B-C3B-CAB	-2.80	121.50	127.18
23	A	405	CLA	O2D-CGD-O1D	-2.80	118.16	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	411	BCR	C24-C23-C22	-2.80	122.02	126.22
37	f	101	HEM	CAD-CBD-CGD	2.80	118.81	113.53
34	D	406	DGD	O2D-C2D-C3D	-2.80	104.10	110.36
23	c	913	CLA	CBA-CAA-C2A	-2.80	107.10	113.95
23	C	510	CLA	C4B-C3B-CAB	-2.80	121.51	127.18
30	B	623	LMT	O1B-C4'-C3'	2.80	114.25	107.17
28	D	405	PL9	C42-C41-C39	-2.80	103.51	112.75
23	B	605	CLA	CMC-C2C-C1C	2.80	128.94	124.95
23	B	605	CLA	C2A-C1A-CHA	-2.80	118.78	123.87
23	b	612	CLA	CMD-C2D-C3D	2.79	130.43	125.16
23	b	607	CLA	C4B-C3B-C2B	-2.79	104.17	107.04
34	c	919	DGD	C4A-C3A-C2A	-2.79	102.93	113.28
23	B	617	CLA	C4C-C3C-C2C	-2.79	102.35	106.93
23	b	604	CLA	C4A-NA-C1A	2.79	110.32	106.38
23	b	608	CLA	O2D-CGD-O1D	-2.79	118.18	123.79
25	b	622	BCR	C3-C4-C5	-2.79	109.22	113.81
23	D	403	CLA	O2D-CGD-O1D	-2.79	118.18	123.79
23	b	611	CLA	C2A-C1A-NA	2.79	114.90	111.33
23	b	612	CLA	C2B-C3B-CAB	2.79	133.03	127.33
23	b	611	CLA	C3B-C4B-CHC	-2.79	120.71	126.00
23	C	510	CLA	C4B-NB-C1B	-2.79	104.43	107.12
23	B	610	CLA	C2D-C3D-CAD	2.79	146.31	134.94
23	c	910	CLA	O2D-CGD-O1D	-2.79	118.19	123.79
23	B	603	CLA	C1C-C2C-C3C	-2.79	103.46	106.96
23	a	410	CLA	C2A-C1A-NA	2.79	114.90	111.33
23	b	612	CLA	C4B-CHC-C1C	-2.78	123.81	127.47
23	C	510	CLA	C4A-NA-C1A	2.78	110.31	106.38
23	D	402	CLA	C3B-C4B-NB	2.78	112.81	109.21
23	C	512	CLA	C3B-CAB-CBB	-2.78	120.19	125.95
23	B	617	CLA	C2A-C1A-CHA	-2.78	118.80	123.87
25	T	101	BCR	C23-C24-C25	-2.78	119.03	127.23
23	b	608	CLA	C4B-CHC-C1C	-2.78	123.81	127.47
23	a	409	CLA	C4B-C3B-CAB	-2.78	121.55	127.18
33	O	303	HTG	C2-C1-S1	2.78	114.10	110.97
23	B	606	CLA	C4C-C3C-C2C	-2.78	102.38	106.93
23	a	409	CLA	C2A-C1A-NA	2.78	114.89	111.33
23	d	402	CLA	CGD-CBD-CHA	-2.78	107.21	113.65
23	C	502	CLA	C5-C3-C2	-2.78	115.72	121.06
23	C	508	CLA	CMC-C2C-C3C	2.78	133.96	126.04
23	A	405	CLA	CMA-C3A-C4A	-2.78	103.53	112.40
23	b	605	CLA	CGD-CBD-CHA	-2.78	107.21	113.65
23	C	502	CLA	O2D-CGD-CBD	2.78	116.95	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	408	PHO	CMB-C2B-C3B	2.78	130.40	125.16
23	c	907	CLA	C2B-C3B-CAB	2.78	133.01	127.33
23	b	614	CLA	C4A-NA-C1A	2.78	110.30	106.38
23	b	618	CLA	C4B-NB-C1B	-2.77	104.45	107.12
23	c	908	CLA	C3B-CAB-CBB	-2.77	120.21	125.95
23	c	904	CLA	CHC-C4B-NB	2.77	129.41	124.70
38	H	101	RRX	C36-C18-C17	2.77	126.86	122.92
23	B	604	CLA	C3C-C4C-NC	2.77	113.49	110.15
23	D	403	CLA	CGD-CBD-CHA	-2.77	107.23	113.65
23	b	610	CLA	C3C-C4C-NC	2.77	113.49	110.15
23	a	411	CLA	C1C-NC-C4C	-2.77	102.53	106.26
34	c	919	DGD	O3G-C1D-C2D	-2.77	104.61	108.15
23	C	511	CLA	CBC-CAC-C3C	-2.77	103.98	112.37
23	b	608	CLA	C4C-C3C-C2C	-2.77	102.40	106.93
23	C	510	CLA	CHB-C4A-NA	2.77	128.24	124.38
23	d	402	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
24	a	412	PHO	CMD-C2D-C1D	2.76	132.70	128.49
24	a	412	PHO	CHD-C4C-C3C	-2.76	118.68	125.42
23	c	907	CLA	C3C-C4C-NC	2.76	113.48	110.15
25	B	620	BCR	C32-C1-C6	-2.76	105.75	110.33
23	c	911	CLA	CHC-C4B-NB	2.76	129.39	124.70
23	C	503	CLA	CMD-C2D-C1D	2.76	131.62	126.16
25	D	404	BCR	C30-C25-C24	2.76	123.34	115.69
23	b	607	CLA	CMB-C2B-C3B	2.76	130.35	125.16
27	C	519	LMG	O8-C9-C8	2.76	116.04	108.80
23	C	511	CLA	C3B-CAB-CBB	-2.75	120.25	125.95
23	A	410	CLA	C3A-C4A-CHB	-2.75	118.60	124.33
25	b	620	BCR	C15-C14-C13	-2.75	123.31	127.29
24	a	412	PHO	C1D-CHD-C4C	-2.75	120.95	126.23
23	C	505	CLA	CMB-C2B-C3B	2.75	130.34	125.16
23	B	612	CLA	C2A-C1A-CHA	-2.75	118.87	123.87
23	b	619	CLA	O2D-CGD-O1D	-2.75	118.27	123.79
23	C	504	CLA	C4B-CHC-C1C	-2.75	123.86	127.47
23	D	402	CLA	C2A-C1A-CHA	-2.75	118.87	123.87
23	c	905	CLA	C7-C6-C5	-2.75	104.95	112.97
28	D	405	PL9	C31-C32-C33	-2.74	103.84	111.64
26	B	621	SQD	O5-C5-C6	2.74	111.77	105.91
23	B	613	CLA	CMB-C2B-C3B	2.74	130.33	125.16
23	B	614	CLA	CBC-CAC-C3C	-2.74	104.07	112.37
25	c	915	BCR	C15-C14-C13	-2.74	123.33	127.29
26	A	412	SQD	O2-C2-C1	2.74	115.99	110.03
23	b	615	CLA	C4A-NA-C1A	2.74	110.24	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	F	101	HEM	C3A-C4A-NA	-2.73	107.67	109.50
25	D	404	BCR	C29-C28-C27	-2.73	104.42	111.46
23	B	606	CLA	C2B-C1B-CHB	-2.73	120.82	126.00
23	c	911	CLA	C4D-ND-C1D	-2.73	103.27	106.57
23	b	613	CLA	C3B-C4B-NB	2.73	112.73	109.21
34	H	102	DGD	O5D-C6D-C5D	-2.73	104.23	108.96
23	b	616	CLA	C3B-C2B-C1B	-2.73	103.67	106.69
23	A	407	CLA	C2B-C1B-CHB	-2.72	120.83	126.00
23	c	903	CLA	C3C-C4C-NC	2.73	113.44	110.15
28	d	405	PL9	C37-C36-C34	-2.72	103.75	112.75
23	c	911	CLA	C4B-C3B-C2B	-2.72	104.24	107.04
23	B	605	CLA	C3B-C2B-C1B	-2.72	103.67	106.69
23	c	909	CLA	C4C-C3C-C2C	-2.72	102.47	106.93
23	b	608	CLA	C2A-C1A-CHA	-2.72	118.92	123.87
24	a	412	PHO	CAA-CBA-CGA	-2.72	105.24	113.24
23	C	505	CLA	CED-O2D-CGD	2.72	122.47	116.00
23	c	908	CLA	O2A-CGA-CBA	2.71	120.21	111.90
23	b	618	CLA	C2B-C3B-CAB	2.71	132.88	127.33
30	z	101	LMT	O5B-C5B-C6B	2.71	113.10	106.34
23	C	505	CLA	CHC-C4B-NB	2.71	129.31	124.70
23	c	906	CLA	C3C-C4C-NC	2.71	113.42	110.15
23	A	410	CLA	CMD-C2D-C3D	2.71	130.27	125.16
23	a	411	CLA	CGD-CBD-CHA	-2.71	107.37	113.65
23	B	616	CLA	C3B-C4B-NB	2.71	112.71	109.21
25	d	404	BCR	C7-C8-C9	-2.71	122.16	126.22
23	C	509	CLA	C4A-NA-C1A	2.71	110.20	106.38
23	b	615	CLA	O2D-CGD-CBD	2.71	116.82	111.34
23	c	912	CLA	C1-O2A-CGA	2.71	124.88	117.00
23	B	616	CLA	O2D-CGD-O1D	-2.71	118.35	123.79
23	B	602	CLA	O2A-CGA-CBA	2.71	120.19	111.90
26	a	401	SQD	C3-C4-C5	2.71	115.03	110.17
26	A	418	SQD	O5-C1-C2	-2.71	104.76	110.30
23	d	403	CLA	C4B-NB-C1B	-2.70	104.52	107.12
25	t	101	BCR	C29-C28-C27	-2.70	104.49	111.46
26	A	418	SQD	C46-O48-C23	2.70	124.71	116.99
23	d	403	CLA	C4D-ND-C1D	-2.70	103.31	106.57
30	b	624	LMT	C2'-C3'-C4'	2.70	115.44	109.59
34	D	406	DGD	O6D-C5D-C6D	2.70	112.03	106.62
23	a	414	CLA	O2D-CGD-O1D	-2.70	118.37	123.79
23	B	615	CLA	C2B-C3B-CAB	2.70	132.85	127.33
23	a	411	CLA	C1-O2A-CGA	2.70	124.84	117.00
34	H	102	DGD	O3G-C3G-C2G	-2.70	104.57	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	416	SQD	O9-S-O7	-2.70	104.08	113.45
25	B	620	BCR	C38-C26-C27	2.70	118.50	113.39
23	b	616	CLA	CMD-C2D-C1D	2.69	131.48	126.16
28	A	414	PL9	C7-C8-C9	-2.69	122.21	126.76
26	A	418	SQD	O48-C23-O10	-2.69	116.44	123.48
23	B	605	CLA	C2A-C1A-NA	2.69	114.78	111.33
26	A	412	SQD	O48-C23-O10	-2.69	116.44	123.48
36	d	409	LHG	O7-C7-C8	2.69	117.27	111.54
23	C	505	CLA	C4B-C3B-C2B	-2.69	104.28	107.04
28	A	414	PL9	C25-C24-C23	-2.69	118.16	123.52
23	b	615	CLA	O2A-CGA-CBA	2.69	120.14	111.90
34	c	917	DGD	C1E-C2E-C3E	-2.69	104.78	109.99
23	C	506	CLA	CMB-C2B-C3B	2.69	130.23	125.16
23	c	913	CLA	CHB-C1B-NB	-2.69	120.14	124.70
34	c	918	DGD	O1G-C1A-O1A	-2.69	116.46	123.48
34	H	102	DGD	O4D-C4D-C3D	-2.69	104.36	110.36
25	D	404	BCR	C30-C25-C26	-2.68	118.70	122.59
24	A	408	PHO	O2D-CGD-CBD	2.68	116.76	111.34
23	c	907	CLA	CHC-C4B-NB	2.68	129.26	124.70
23	A	407	CLA	CMD-C2D-C1D	2.68	131.46	126.16
26	A	412	SQD	O47-C7-O49	-2.68	116.51	123.66
23	b	606	CLA	C2A-C1A-CHA	-2.68	119.00	123.87
34	H	102	DGD	CGA-CFA-CEA	2.68	120.59	112.94
25	A	411	BCR	C27-C26-C25	2.68	126.39	122.86
23	B	616	CLA	C4C-C3C-C2C	-2.68	102.54	106.93
23	B	605	CLA	C5-C3-C2	-2.68	115.92	121.06
27	a	418	LMG	O1-C1-C2	2.67	111.58	108.15
23	c	903	CLA	C4B-NB-C1B	-2.67	104.55	107.12
23	c	914	CLA	C1-O2A-CGA	2.67	124.77	117.00
23	C	511	CLA	C4B-C3B-C2B	-2.67	104.30	107.04
26	a	401	SQD	O48-C46-C45	2.67	115.82	108.80
26	a	416	SQD	C44-O6-C1	-2.67	108.44	113.80
23	B	611	CLA	C4-C3-C5	2.67	119.44	115.39
27	c	921	LMG	O8-C28-C29	2.67	120.06	111.90
23	B	616	CLA	CAC-C3C-C2C	2.67	132.31	127.50
23	c	907	CLA	C1D-CHD-C4C	-2.66	118.47	122.60
25	A	411	BCR	C35-C13-C14	-2.66	119.12	122.92
23	c	907	CLA	CED-O2D-CGD	2.66	122.34	116.00
23	B	602	CLA	C1D-CHD-C4C	-2.66	118.47	122.60
36	D	408	LHG	C6-O8-C23	2.66	124.59	116.99
23	B	603	CLA	CMB-C2B-C3B	2.66	130.17	125.16
23	A	406	CLA	CHC-C1C-C2C	-2.66	119.37	126.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	O2A-CGA-O1A	-2.66	116.53	123.48
26	a	416	SQD	O47-C7-O49	-2.66	116.57	123.66
23	b	604	CLA	C1D-CHD-C4C	-2.66	118.48	122.60
23	B	611	CLA	CHB-C1B-NB	-2.66	120.19	124.70
23	B	603	CLA	CHC-C4B-NB	2.66	129.21	124.70
23	b	610	CLA	C3B-C4B-NB	2.66	112.64	109.21
34	c	918	DGD	O3D-C3D-C2D	-2.65	104.43	110.36
28	D	405	PL9	C12-C13-C14	-2.65	122.07	127.81
23	b	616	CLA	O2A-CGA-CBA	2.66	120.03	111.90
23	D	403	CLA	C6-C7-C8	-2.66	107.18	115.44
23	b	605	CLA	C3B-C4B-CHC	-2.65	120.97	126.00
26	a	416	SQD	O5-C5-C6	2.65	111.58	105.91
23	b	610	CLA	C4C-C3C-C2C	-2.65	102.58	106.93
23	C	504	CLA	C2A-C1A-NA	2.65	114.72	111.33
27	a	418	LMG	O7-C10-O9	-2.65	116.60	123.66
34	H	102	DGD	O6E-C5E-C6E	2.65	112.94	106.34
25	c	915	BCR	C38-C26-C25	-2.65	121.51	124.50
23	B	603	CLA	CGD-CBD-CHA	-2.65	107.51	113.65
23	c	911	CLA	C3C-C4C-NC	2.65	113.34	110.15
23	B	604	CLA	C2B-C3B-CAB	2.65	132.74	127.33
23	A	407	CLA	CAC-C3C-C2C	-2.65	122.73	127.50
34	d	406	DGD	O1G-C1A-C2A	2.65	120.00	111.90
28	A	414	PL9	C17-C18-C19	-2.64	122.09	127.81
30	A	419	LMT	O5'-C1'-C2'	-2.64	104.89	110.30
27	Z	101	LMG	O8-C28-C29	2.64	119.99	111.90
23	c	910	CLA	CED-O2D-CGD	2.64	122.29	116.00
23	a	411	CLA	CHC-C1C-C2C	-2.64	119.42	126.51
23	c	912	CLA	CMC-C2C-C1C	2.64	128.71	124.95
24	A	408	PHO	CHC-C1C-C2C	-2.64	118.46	124.93
25	c	916	BCR	C11-C10-C9	-2.64	123.48	127.29
23	b	613	CLA	CMD-C2D-C3D	2.64	130.13	125.16
34	C	516	DGD	C1E-O6E-C5E	2.64	118.83	113.73
25	c	916	BCR	C15-C16-C17	-2.64	117.64	123.45
30	b	624	LMT	C3'-C4'-C5'	2.63	116.75	110.86
23	b	614	CLA	C2A-C1A-NA	2.64	114.71	111.33
26	B	621	SQD	O47-C7-C8	2.63	117.15	111.54
23	c	912	CLA	C3B-C4B-NB	2.63	112.61	109.21
23	b	615	CLA	C1C-NC-C4C	-2.63	102.71	106.26
23	b	617	CLA	CAC-C3C-C4C	2.63	128.80	124.85
23	b	609	CLA	C4B-C3B-C2B	-2.63	104.33	107.04
26	A	418	SQD	O48-C46-C45	2.63	115.72	108.80
23	C	509	CLA	C3B-C4B-NB	2.63	112.61	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	h	102	DGD	O2G-C1B-C2B	2.63	117.15	111.54
23	b	618	CLA	C4B-C3B-CAB	-2.63	121.85	127.18
23	B	603	CLA	CAA-CBA-CGA	-2.63	105.49	113.24
23	b	606	CLA	C3C-C4C-NC	2.63	113.32	110.15
23	a	411	CLA	C3A-C2A-C1A	-2.63	97.43	101.70
23	b	610	CLA	O2D-CGD-O1D	-2.63	118.51	123.79
23	d	403	CLA	CMD-C2D-C1D	2.63	131.35	126.16
23	B	608	CLA	CMA-C3A-C4A	-2.63	104.00	112.40
36	l	101	LHG	O7-C7-C8	2.63	117.14	111.54
23	b	617	CLA	O2A-CGA-CBA	2.62	119.93	111.90
23	b	605	CLA	C3A-C4A-CHB	-2.62	118.88	124.33
23	A	407	CLA	C4B-CHC-C1C	-2.62	124.02	127.47
23	c	905	CLA	C3B-CAB-CBB	-2.62	120.52	125.95
23	C	503	CLA	CGD-CBD-CHA	-2.62	107.57	113.65
23	C	513	CLA	O2A-CGA-CBA	2.62	119.92	111.90
23	c	910	CLA	C4B-CHC-C1C	-2.62	124.02	127.47
27	c	920	LMG	O8-C9-C8	2.62	115.68	108.80
23	a	409	CLA	O2D-CGD-O1D	-2.62	118.53	123.79
23	b	619	CLA	C2A-C1A-CHA	-2.62	119.10	123.87
23	B	610	CLA	CHC-C4B-NB	2.62	129.15	124.70
23	b	613	CLA	C4B-NB-C1B	-2.62	104.60	107.12
23	c	907	CLA	C4B-C3B-CAB	-2.62	121.88	127.18
23	c	905	CLA	C4C-C3C-C2C	-2.62	102.64	106.93
28	a	419	PL9	C17-C18-C19	-2.61	122.16	127.81
23	c	902	CLA	CBC-CAC-C3C	-2.61	104.45	112.37
23	b	610	CLA	CMD-C2D-C3D	2.61	130.09	125.16
23	C	506	CLA	C1C-NC-C4C	-2.61	102.74	106.26
23	b	608	CLA	O2A-C1-C2	-2.61	102.14	108.12
23	D	402	CLA	CMC-C2C-C1C	2.61	128.67	124.95
23	a	409	CLA	C3B-C4B-NB	2.61	112.58	109.21
23	b	606	CLA	O2D-CGD-CBD	2.61	116.61	111.34
25	d	404	BCR	C30-C25-C24	2.61	122.92	115.69
25	B	620	BCR	C2-C1-C6	2.61	114.53	110.37
27	b	623	LMG	C13-C12-C11	2.61	122.94	113.28
23	c	903	CLA	C3B-CAB-CBB	-2.61	120.55	125.95
23	b	610	CLA	CMB-C2B-C3B	2.61	130.08	125.16
24	a	413	PHO	O2A-CGA-O1A	-2.61	116.66	123.48
30	M	102	LMT	O1'-C1-C2	-2.61	99.77	109.79
23	b	605	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
25	A	411	BCR	C33-C5-C6	-2.61	121.55	124.50
30	B	623	LMT	C1B-C2B-C3B	-2.60	104.94	109.99
23	b	617	CLA	CMD-C2D-C1D	2.60	131.31	126.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	922	LMT	O5'-C5'-C6'	2.60	112.83	106.34
23	C	512	CLA	CED-O2D-CGD	2.60	122.20	116.00
23	b	605	CLA	CMA-C3A-C4A	-2.60	104.09	112.40
34	C	516	DGD	CDB-CEB-CFB	-2.60	103.27	113.73
23	C	501	CLA	CMD-C2D-C3D	2.60	130.06	125.16
23	d	402	CLA	C2B-C1B-CHB	-2.60	121.08	126.00
23	D	402	CLA	OBD-CAD-C3D	-2.60	122.91	128.15
36	d	408	LHG	C32-C31-C30	-2.60	100.78	114.56
23	c	903	CLA	C4B-CHC-C1C	-2.60	124.06	127.47
23	c	907	CLA	C2A-C1A-CHA	-2.59	119.15	123.87
23	b	614	CLA	C1D-CHD-C4C	-2.59	118.58	122.60
23	B	614	CLA	CAC-C3C-C4C	2.59	128.74	124.85
23	b	613	CLA	O2A-CGA-O1A	-2.59	116.71	123.48
23	B	607	CLA	C3B-C2B-C1B	-2.59	103.82	106.69
23	B	602	CLA	C3C-C4C-NC	2.59	113.27	110.15
34	C	516	DGD	O6E-C5E-C6E	2.59	112.79	106.34
24	a	413	PHO	CBA-CAA-C2A	-2.59	107.62	113.95
23	b	616	CLA	CMB-C2B-C3B	2.59	130.03	125.16
23	B	612	CLA	C1C-NC-C4C	-2.59	102.77	106.26
23	c	910	CLA	C4A-NA-C1A	2.59	110.03	106.38
23	D	403	CLA	C2A-C1A-NA	2.59	114.64	111.33
23	D	403	CLA	CHC-C4B-NB	2.59	129.09	124.70
23	b	616	CLA	C2A-C1A-NA	2.58	114.64	111.33
23	c	910	CLA	C2B-C3B-CAB	2.58	132.61	127.33
23	b	608	CLA	C4B-C3B-C2B	-2.58	104.39	107.04
23	B	605	CLA	O2A-CGA-O1A	-2.58	116.74	123.48
23	c	910	CLA	C4B-C3B-C2B	-2.58	104.39	107.04
23	D	403	CLA	C3B-CAB-CBB	-2.57	120.62	125.95
34	c	917	DGD	O2G-C1B-O1B	-2.57	116.80	123.66
36	L	101	LHG	O8-C23-O10	-2.57	116.76	123.48
25	T	101	BCR	C23-C22-C21	-2.57	115.02	118.98
23	b	604	CLA	C3B-CAB-CBB	-2.57	120.62	125.95
23	B	614	CLA	C4-C3-C5	2.57	119.30	115.39
31	B	633	GOL	O3-C3-C2	-2.57	98.94	110.37
34	d	406	DGD	C1G-O1G-C1A	2.57	124.33	116.99
25	k	102	BCR	C24-C23-C22	-2.57	122.37	126.22
23	C	512	CLA	OBD-CAD-C3D	-2.57	122.96	128.15
23	A	405	CLA	C4B-CHC-C1C	-2.57	124.09	127.47
26	a	416	SQD	O5-C1-O6	2.57	116.04	109.93
23	b	617	CLA	C4D-CHA-C1A	-2.56	112.89	120.32
23	a	409	CLA	O2A-CGA-O1A	-2.56	116.78	123.48
26	D	407	SQD	C3-C4-C5	2.56	114.77	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	m	101	LMT	C1'-O5'-C5'	-2.56	108.78	113.73
25	d	404	BCR	C34-C9-C10	-2.56	119.27	122.92
34	h	102	DGD	O3G-C3G-C2G	-2.56	104.90	110.99
23	B	604	CLA	C4-C3-C5	2.56	119.27	115.39
23	b	607	CLA	C3B-C4B-NB	2.56	112.52	109.21
26	a	416	SQD	C5-C6-S	-2.56	110.83	114.40
23	A	406	CLA	C4B-C3B-C2B	-2.55	104.42	107.04
25	K	101	BCR	C15-C16-C17	-2.55	117.83	123.45
25	c	915	BCR	C11-C10-C9	-2.55	123.60	127.29
23	A	405	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
23	c	912	CLA	O2A-CGA-CBA	2.55	119.72	111.90
23	b	616	CLA	C11-C10-C8	-2.55	107.50	115.44
23	C	504	CLA	C1-O2A-CGA	2.55	124.43	117.00
23	C	502	CLA	CHB-C4A-NA	2.55	127.94	124.38
23	C	501	CLA	C4B-C3B-C2B	-2.55	104.42	107.04
23	b	615	CLA	C2D-C3D-CAD	2.55	145.34	134.94
23	B	604	CLA	C2B-C1B-CHB	-2.55	121.17	126.00
28	d	405	PL9	C53-C6-C1	2.55	121.03	114.99
23	B	603	CLA	CMD-C2D-C3D	2.54	129.96	125.16
38	h	101	RRX	C38-C26-C25	-2.54	121.62	124.50
24	A	408	PHO	C1C-C2C-C3C	-2.54	103.43	106.55
23	D	403	CLA	C4A-NA-C1A	2.55	109.97	106.38
36	d	408	LHG	O7-C7-C8	2.54	116.96	111.54
23	c	905	CLA	C4B-CHC-C1C	-2.54	124.12	127.47
23	b	607	CLA	C2B-C3B-CAB	2.54	132.53	127.33
34	c	918	DGD	O5D-C1E-C2E	-2.54	104.90	108.15
30	A	419	LMT	C1-O1'-C1'	2.54	118.39	113.91
23	b	612	CLA	C4B-C3B-C2B	-2.54	104.43	107.04
23	b	607	CLA	C4B-CHC-C1C	-2.54	124.13	127.47
23	B	609	CLA	O2A-CGA-O1A	-2.54	116.85	123.48
24	a	412	PHO	CHD-C4C-NC	-2.54	124.15	128.68
23	C	507	CLA	CHC-C4B-NB	2.54	129.01	124.70
25	k	101	BCR	C8-C9-C10	-2.54	115.07	118.98
26	A	412	SQD	C5-C6-S	-2.54	110.86	114.40
38	H	101	RRX	C10-C11-C12	-2.54	114.72	123.23
23	b	615	CLA	CHC-C4B-NB	2.54	129.01	124.70
27	c	921	LMG	O8-C9-C8	2.53	115.46	108.80
23	b	605	CLA	C1D-CHD-C4C	-2.54	118.67	122.60
23	B	605	CLA	C4B-C3B-C2B	-2.53	104.44	107.04
23	c	910	CLA	OBD-CAD-CBD	2.54	129.76	125.94
23	A	406	CLA	C3A-C2A-C1A	-2.53	97.59	101.70
23	C	511	CLA	C3C-C4C-NC	2.53	113.20	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	409	LHG	O8-C23-C24	2.53	119.65	111.90
23	B	609	CLA	C4D-ND-C1D	-2.53	103.51	106.57
33	B	624	HTG	O3-C3-C4	-2.53	104.70	110.36
23	B	610	CLA	CGD-CBD-CHA	-2.53	107.78	113.65
23	C	512	CLA	CMB-C2B-C3B	2.53	129.93	125.16
26	L	103	SQD	C4-C3-C2	2.53	115.46	110.80
25	K	101	BCR	C23-C22-C21	-2.53	115.09	118.98
23	C	513	CLA	CMB-C2B-C3B	2.52	129.92	125.16
23	b	614	CLA	C3C-C4C-NC	2.52	113.19	110.15
23	d	402	CLA	CHB-C4A-NA	2.52	127.90	124.38
27	a	418	LMG	O8-C28-C29	2.52	119.62	111.90
23	C	502	CLA	CMD-C2D-C1D	2.52	131.14	126.16
23	C	504	CLA	CGD-CBD-CHA	-2.52	107.81	113.65
23	B	617	CLA	C1C-NC-C4C	-2.52	102.86	106.26
23	c	903	CLA	CAC-C3C-C4C	2.52	128.63	124.85
34	c	917	DGD	C1D-O6D-C5D	-2.52	108.86	113.73
23	B	602	CLA	C4B-C3B-C2B	-2.52	104.45	107.04
34	H	102	DGD	O3G-C1D-C2D	-2.52	104.93	108.15
23	B	611	CLA	C1D-CHD-C4C	-2.52	118.70	122.60
23	b	607	CLA	CED-O2D-CGD	2.52	121.99	116.00
23	B	603	CLA	C4B-C3B-CAB	-2.52	122.08	127.18
23	c	912	CLA	O2A-C1-C2	-2.52	102.36	108.12
23	B	602	CLA	C3B-C4B-NB	2.52	112.46	109.21
26	B	621	SQD	O5-C5-C4	-2.51	105.06	109.73
23	d	403	CLA	CED-O2D-CGD	2.51	121.98	116.00
23	C	512	CLA	C2B-C3B-CAB	2.51	132.47	127.33
23	c	902	CLA	C3B-CAB-CBB	-2.51	120.75	125.95
23	b	609	CLA	C3B-C4B-CHC	-2.51	121.24	126.00
23	D	403	CLA	C2A-C1A-CHA	-2.51	119.30	123.87
23	C	502	CLA	C3A-C4A-CHB	-2.51	119.11	124.33
23	B	603	CLA	C2A-C1A-NA	2.51	114.55	111.33
23	A	407	CLA	C3A-C4A-NA	2.51	113.84	110.81
23	A	407	CLA	C4B-NB-C1B	-2.51	104.70	107.12
30	M	101	LMT	O5'-C5'-C6'	2.51	112.59	106.34
23	D	403	CLA	O2D-CGD-CBD	2.51	116.41	111.34
23	B	607	CLA	C4D-ND-C1D	-2.51	103.54	106.57
23	C	508	CLA	C4B-CHC-C1C	-2.51	124.17	127.47
23	B	606	CLA	CMB-C2B-C3B	2.51	129.88	125.16
23	b	619	CLA	C3B-C4B-NB	2.51	112.45	109.21
23	B	613	CLA	CED-O2D-CGD	2.50	121.96	116.00
23	B	615	CLA	C4C-C3C-C2C	-2.51	102.82	106.93
23	d	403	CLA	CMB-C2B-C1B	2.50	132.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	914	CLA	CHC-C4B-NB	2.50	128.95	124.70
23	C	512	CLA	C3C-C4C-NC	2.50	113.17	110.15
34	d	406	DGD	C4D-C3D-C2D	2.50	115.42	110.80
27	B	622	LMG	C9-C8-C7	-2.50	106.11	111.86
27	C	519	LMG	C8-O7-C10	-2.50	111.97	117.86
33	B	631	HTG	O5-C5-C6	2.50	112.57	106.34
30	C	520	LMT	O1'-C1'-C2'	2.50	111.36	108.15
24	A	408	PHO	C4B-NB-C1B	-2.50	103.77	108.29
28	d	405	PL9	C16-C14-C13	-2.50	116.26	121.06
23	b	611	CLA	CAC-C3C-C4C	2.50	128.60	124.85
23	C	502	CLA	C2B-C3B-CAB	2.50	132.44	127.33
36	d	407	LHG	O3-C3-C2	-2.50	100.47	108.54
23	B	605	CLA	CAC-C3C-C4C	2.50	128.60	124.85
23	b	613	CLA	O2D-CGD-O1D	-2.50	118.78	123.79
23	B	613	CLA	C3A-C4A-NA	2.50	113.83	110.81
23	b	614	CLA	C4B-NB-C1B	-2.50	104.72	107.12
25	b	622	BCR	C8-C7-C6	-2.50	119.87	127.23
33	C	522	HTG	O5-C5-C4	2.49	114.37	109.73
23	b	610	CLA	C1C-C2C-C3C	-2.49	103.82	106.96
23	c	908	CLA	CBC-CAC-C3C	-2.49	104.82	112.37
23	A	410	CLA	C4B-C3B-C2B	-2.49	104.48	107.04
34	c	918	DGD	O1G-C1A-C2A	2.49	119.52	111.90
30	B	623	LMT	O4'-C4B-C3B	-2.49	104.79	110.36
23	B	608	CLA	CGD-CBD-CAD	-2.49	102.42	110.79
23	D	403	CLA	C4B-NB-C1B	-2.49	104.72	107.12
37	v	201	HEM	CAD-CBD-CGD	-2.49	108.83	113.53
23	B	609	CLA	O1D-CGD-CBD	-2.49	119.37	124.45
23	C	510	CLA	C1C-C2C-C3C	-2.49	103.83	106.96
23	C	504	CLA	C2B-C3B-CAB	2.49	132.42	127.33
28	d	405	PL9	C25-C24-C26	2.49	119.16	115.39
34	D	406	DGD	O3G-C3G-C2G	2.49	116.90	110.99
23	B	604	CLA	CMD-C2D-C3D	2.49	129.85	125.16
23	b	616	CLA	C1-O2A-CGA	2.49	124.23	117.00
23	C	509	CLA	CHB-C4A-NA	2.49	127.85	124.38
23	B	604	CLA	C4B-CHC-C1C	-2.48	124.20	127.47
24	a	413	PHO	CHD-C4C-C3C	-2.48	119.36	125.42
23	b	605	CLA	C4B-C3B-CAB	-2.48	122.15	127.18
23	d	403	CLA	C5-C3-C2	-2.48	116.29	121.06
23	C	511	CLA	C3A-C2A-C1A	2.48	105.73	101.70
23	d	402	CLA	C2D-C3D-CAD	2.48	145.05	134.94
26	A	412	SQD	C44-O6-C1	-2.48	108.83	113.80
23	b	615	CLA	C4B-C3B-C2B	-2.48	104.49	107.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	518	DGD	C4B-C3B-C2B	-2.48	104.10	113.28
23	A	410	CLA	O2A-CGA-O1A	-2.48	117.00	123.48
23	b	614	CLA	C3B-CAB-CBB	-2.48	120.82	125.95
23	b	615	CLA	CMC-C2C-C1C	2.48	128.48	124.95
25	k	101	BCR	C23-C24-C25	-2.48	119.93	127.23
23	c	910	CLA	CMD-C2D-C1D	2.48	131.05	126.16
23	B	607	CLA	O2A-CGA-O1A	-2.48	117.01	123.48
23	C	504	CLA	CMC-C2C-C1C	2.48	128.48	124.95
23	d	403	CLA	CBC-CAC-C3C	-2.47	104.88	112.37
23	C	511	CLA	C4-C3-C5	2.47	119.14	115.39
23	c	910	CLA	C3A-C4A-CHB	-2.47	119.19	124.33
23	c	909	CLA	C2D-C3D-CAD	2.47	145.02	134.94
23	c	906	CLA	C4-C3-C5	2.47	119.14	115.39
23	B	609	CLA	CHC-C1C-C2C	-2.47	119.87	126.51
24	a	412	PHO	C4B-C3B-C2B	-2.47	105.17	106.90
24	A	409	PHO	CED-O2D-CGD	2.47	121.88	116.00
23	A	410	CLA	C4B-C3B-CAB	-2.47	122.17	127.18
23	B	611	CLA	C2A-C1A-NA	2.47	114.50	111.33
23	C	513	CLA	CMC-C2C-C1C	2.47	128.47	124.95
27	B	622	LMG	C35-C34-C33	-2.47	101.46	114.56
37	F	101	HEM	CAD-CBD-CGD	2.47	118.18	113.53
23	b	610	CLA	C3B-CAB-CBB	-2.47	120.84	125.95
23	b	618	CLA	C4A-NA-C1A	2.47	109.86	106.38
23	A	405	CLA	C3C-C4C-NC	2.47	113.12	110.15
27	C	519	LMG	O7-C10-O9	-2.47	117.08	123.66
23	c	914	CLA	C3C-C4C-NC	2.46	113.12	110.15
23	A	406	CLA	O2D-CGD-O1D	-2.46	118.84	123.79
23	c	904	CLA	CBD-CHA-C1A	2.46	131.99	128.77
25	b	620	BCR	C33-C5-C4	2.46	118.06	113.39
23	b	605	CLA	O2A-CGA-CBA	2.46	119.43	111.90
23	C	510	CLA	CMD-C2D-C1D	2.46	131.02	126.16
23	C	513	CLA	C3B-CAB-CBB	-2.46	120.86	125.95
23	C	502	CLA	C3C-C4C-NC	2.46	113.11	110.15
23	B	613	CLA	CAA-CBA-CGA	-2.46	105.99	113.24
23	b	606	CLA	C2A-C1A-NA	2.46	114.48	111.33
23	B	607	CLA	C1-O2A-CGA	2.46	124.15	117.00
28	a	419	PL9	C11-C9-C8	-2.46	116.34	121.06
23	c	909	CLA	C4-C3-C5	2.46	119.12	115.39
23	B	608	CLA	C2A-C1A-CHA	-2.46	119.40	123.87
25	D	404	BCR	C32-C1-C6	2.46	114.40	110.33
34	c	918	DGD	CGB-CFB-CEB	-2.45	105.93	112.94
23	c	910	CLA	C4D-ND-C1D	-2.45	103.60	106.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	913	CLA	C6-C5-C3	-2.45	107.03	112.62
24	A	408	PHO	C2B-C1B-NB	2.45	114.84	106.15
23	B	617	CLA	CAA-C2A-C1A	-2.45	106.02	112.51
23	C	512	CLA	C2A-C1A-CHA	-2.45	119.41	123.87
25	k	102	BCR	C3-C4-C5	-2.45	109.79	113.81
24	A	408	PHO	O2D-CGD-O1D	-2.45	118.87	123.79
23	b	614	CLA	CMD-C2D-C3D	2.45	129.77	125.16
23	C	510	CLA	CHC-C4B-NB	2.45	128.86	124.70
30	m	102	LMT	O2'-C2'-C1'	2.45	115.36	110.03
24	a	413	PHO	C1C-C2C-C3C	-2.45	103.55	106.55
23	c	910	CLA	O1D-CGD-CBD	-2.45	119.45	124.45
23	a	411	CLA	C4C-C3C-C2C	-2.44	102.92	106.93
23	a	414	CLA	CHC-C1C-C2C	-2.45	119.94	126.51
25	D	404	BCR	C15-C14-C13	-2.44	123.75	127.29
26	D	407	SQD	C5-C6-S	-2.44	110.98	114.40
23	a	414	CLA	C4B-NB-C1B	-2.44	104.77	107.12
23	c	904	CLA	CGD-CBD-CHA	-2.44	107.99	113.65
36	d	408	LHG	C13-C12-C11	-2.44	101.59	114.56
34	h	102	DGD	O6E-C1E-C2E	-2.44	105.31	110.30
23	c	905	CLA	CAA-C2A-C1A	-2.44	106.04	112.51
23	C	502	CLA	CHC-C4B-NB	2.44	128.85	124.70
23	C	513	CLA	C3C-C4C-NC	2.44	113.09	110.15
23	c	906	CLA	C3B-C4B-CHC	-2.44	121.38	126.00
36	d	408	LHG	O7-C7-O9	-2.44	117.16	123.66
34	d	406	DGD	O6D-C5D-C4D	2.44	112.68	108.67
25	A	411	BCR	C35-C13-C12	2.44	122.03	118.09
23	C	508	CLA	C4D-ND-C1D	-2.43	103.63	106.57
30	a	402	LMT	O4'-C4B-C3B	-2.43	104.92	110.36
23	c	909	CLA	CGD-CBD-CHA	-2.43	108.01	113.65
23	b	614	CLA	C14-C13-C15	-2.44	101.53	111.05
27	Z	101	LMG	O1-C7-C8	2.43	116.78	110.99
23	C	505	CLA	C2A-C1A-NA	2.43	114.45	111.33
23	a	411	CLA	CHD-C4C-NC	2.43	125.98	124.28
23	b	605	CLA	C2B-C1B-CHB	-2.43	121.39	126.00
27	d	410	LMG	O8-C28-C29	2.43	119.34	111.90
23	c	907	CLA	C6-C5-C3	-2.43	107.08	112.62
23	b	604	CLA	C2A-C1A-CHA	-2.43	119.45	123.87
23	d	402	CLA	C3A-C4A-NA	2.43	113.74	110.81
23	a	411	CLA	CMD-C2D-C1D	2.43	130.95	126.16
23	b	617	CLA	CHC-C4B-NB	2.42	128.82	124.70
23	C	506	CLA	C4B-C3B-CAB	-2.42	122.27	127.18
23	c	911	CLA	C2B-C3B-CAB	2.42	132.28	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	625	LMT	C1'-C2'-C3'	2.42	114.68	109.99
25	C	514	BCR	C23-C22-C21	-2.43	115.24	118.98
23	B	617	CLA	CBC-CAC-C3C	-2.42	105.03	112.37
23	B	614	CLA	C14-C13-C15	-2.42	101.57	111.05
23	D	402	CLA	CHB-C4A-NA	-2.42	121.00	124.38
23	c	911	CLA	C3B-C4B-NB	2.42	112.34	109.21
23	B	616	CLA	CHB-C1B-NB	-2.42	120.59	124.70
25	c	916	BCR	C8-C7-C6	-2.42	120.09	127.23
25	t	101	BCR	C23-C24-C25	-2.42	120.09	127.23
37	V	201	HEM	C4A-NA-C1A	-2.42	104.92	107.93
28	a	419	PL9	C53-C6-C1	2.42	120.73	114.99
23	c	904	CLA	CMB-C2B-C3B	2.42	129.72	125.16
34	H	102	DGD	C2G-O2G-C1B	-2.42	112.17	117.86
23	b	612	CLA	CHC-C4B-NB	2.42	128.81	124.70
36	D	408	LHG	O7-C7-O9	-2.42	117.21	123.66
30	B	623	LMT	O2'-C2'-C1'	2.42	115.29	110.03
27	c	920	LMG	C8-O7-C10	-2.42	112.17	117.86
23	b	617	CLA	C1-O2A-CGA	2.42	124.02	117.00
23	C	506	CLA	C4B-CHC-C1C	-2.42	124.29	127.47
34	D	406	DGD	O2G-C1B-O1B	-2.42	117.22	123.66
23	a	409	CLA	C2B-C3B-CAB	2.42	132.27	127.33
23	C	508	CLA	C2B-C3B-CAB	2.41	132.26	127.33
23	a	409	CLA	C1D-CHD-C4C	-2.41	118.86	122.60
23	b	609	CLA	C3C-C4C-NC	2.41	113.06	110.15
34	h	102	DGD	C6D-O5D-C1E	2.41	118.64	113.80
25	a	415	BCR	C15-C14-C13	-2.41	123.80	127.29
23	b	619	CLA	C1C-C2C-C3C	-2.41	103.93	106.96
36	D	409	LHG	C34-C33-C32	-2.41	101.76	114.56
23	d	403	CLA	C2A-C1A-CHA	-2.41	119.49	123.87
23	C	502	CLA	C4B-C3B-C2B	-2.41	104.56	107.04
25	B	620	BCR	C23-C24-C25	-2.41	120.12	127.23
23	C	510	CLA	CMB-C2B-C3B	2.41	129.70	125.16
23	c	905	CLA	C16-C15-C13	2.41	122.94	115.44
23	A	405	CLA	C2B-C3B-CAB	2.41	132.25	127.33
25	A	411	BCR	C20-C21-C22	-2.41	123.81	127.29
23	c	913	CLA	C4A-NA-C1A	2.41	109.77	106.38
25	T	101	BCR	C24-C23-C22	-2.41	122.61	126.22
23	c	902	CLA	CHC-C4B-NB	2.41	128.79	124.70
23	c	909	CLA	CHB-C1B-NB	-2.41	120.62	124.70
37	F	101	HEM	CMC-C2C-C3C	2.41	129.95	124.26
23	C	509	CLA	CHD-C4C-NC	2.40	125.96	124.28
30	J	102	LMT	O1'-C1'-C2'	2.40	111.23	108.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C3B-C4B-NB	2.40	112.31	109.21
25	d	404	BCR	C21-C20-C19	-2.40	115.17	123.23
23	C	504	CLA	CHC-C4B-NB	2.40	128.78	124.70
27	c	920	LMG	O8-C28-O10	-2.40	117.21	123.48
23	C	502	CLA	C6-C5-C3	-2.40	107.15	112.62
23	C	501	CLA	CGD-CBD-CHA	-2.40	108.09	113.65
23	b	619	CLA	C2D-C3D-CAD	2.40	144.71	134.94
23	b	616	CLA	C4C-C3C-C2C	-2.40	103.00	106.93
23	C	501	CLA	CMB-C2B-C1B	2.40	132.15	128.46
23	b	617	CLA	CBC-CAC-C3C	-2.40	105.11	112.37
24	a	413	PHO	C2B-C1B-NB	2.39	114.64	106.15
23	B	616	CLA	C2B-C3B-CAB	2.39	132.22	127.33
24	A	409	PHO	C16-C15-C13	-2.39	107.99	115.44
23	c	903	CLA	C4A-NA-C1A	2.40	109.76	106.38
23	B	611	CLA	CMD-C2D-C1D	2.40	130.89	126.16
23	a	409	CLA	C4D-ND-C1D	-2.39	103.67	106.57
23	C	508	CLA	C2A-C1A-CHA	-2.39	119.52	123.87
23	B	614	CLA	C2A-C1A-NA	2.39	114.39	111.33
23	C	504	CLA	C3B-C4B-NB	2.39	112.30	109.21
25	t	101	BCR	C2-C3-C4	-2.39	105.30	111.46
23	b	618	CLA	C2B-C1B-CHB	-2.39	121.47	126.00
23	b	612	CLA	C7-C6-C5	-2.39	106.00	112.97
34	c	919	DGD	O5D-C6D-C5D	-2.39	104.82	108.96
34	C	516	DGD	C3D-C4D-C5D	-2.39	105.89	110.17
23	b	604	CLA	C3B-C4B-CHC	-2.39	121.47	126.00
23	b	614	CLA	C16-C15-C13	2.38	122.86	115.44
23	C	507	CLA	O2A-CGA-O1A	-2.38	117.25	123.48
23	A	407	CLA	CMB-C2B-C1B	-2.38	124.80	128.46
23	A	407	CLA	CHC-C4B-NB	2.38	128.75	124.70
23	c	906	CLA	C4-C3-C2	-2.38	118.78	123.52
23	B	617	CLA	CGD-CBD-CHA	-2.38	108.13	113.65
23	b	610	CLA	CGD-CBD-CAD	-2.38	102.78	110.79
23	b	617	CLA	CED-O2D-CGD	2.38	121.67	116.00
24	a	413	PHO	CAA-C2A-C1A	-2.38	106.48	112.78
23	b	619	CLA	CED-O2D-CGD	2.38	121.67	116.00
27	Z	101	LMG	O6-C5-C4	2.38	114.15	109.73
23	B	610	CLA	C2A-C1A-CHA	-2.38	119.54	123.87
25	b	620	BCR	C20-C21-C22	-2.38	123.85	127.29
23	b	607	CLA	CMD-C2D-C3D	2.38	129.64	125.16
23	c	912	CLA	CBC-CAC-C3C	-2.38	105.17	112.37
23	B	602	CLA	C4B-NB-C1B	-2.38	104.83	107.12
23	B	613	CLA	C2D-C3D-CAD	2.38	144.63	134.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	101	LMG	O8-C28-O10	-2.38	117.27	123.48
23	b	612	CLA	C2A-C1A-CHA	-2.38	119.55	123.87
23	c	907	CLA	C4D-CHA-C1A	-2.37	113.44	120.32
23	B	615	CLA	C1-C2-C3	-2.37	122.11	126.23
34	d	406	DGD	O2G-C1B-O1B	-2.37	117.33	123.66
23	a	411	CLA	O2D-CGD-O1D	-2.37	119.03	123.79
23	b	604	CLA	C2B-C1B-CHB	-2.37	121.50	126.00
23	C	510	CLA	O2A-CGA-O1A	-2.37	117.28	123.48
23	c	908	CLA	C3B-C4B-NB	2.37	112.28	109.21
26	A	412	SQD	O3-C3-C4	2.37	115.65	110.36
23	c	907	CLA	O2D-CGD-CBD	2.37	116.13	111.34
23	a	410	CLA	OBD-CAD-C3D	-2.37	123.36	128.15
23	c	911	CLA	O2A-C1-C2	-2.37	102.69	108.12
23	b	605	CLA	C2B-C3B-CAB	2.37	132.17	127.33
23	b	607	CLA	C4C-C3C-C2C	-2.37	103.05	106.93
38	h	101	RRX	C7-C8-C9	-2.37	122.67	126.22
23	c	904	CLA	C1D-CHD-C4C	-2.37	118.93	122.60
25	b	620	BCR	C39-C30-C25	2.36	114.24	110.33
23	a	411	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
23	a	411	CLA	C4B-C3B-C2B	-2.37	104.61	107.04
23	a	411	CLA	CMD-C2D-C3D	2.37	129.62	125.16
33	B	625	HTG	C1-C2-C3	2.37	115.66	110.72
23	c	913	CLA	CHC-C4B-NB	2.36	128.72	124.70
23	B	612	CLA	C3A-C2A-C1A	-2.36	97.87	101.70
23	c	910	CLA	C3B-CAB-CBB	-2.36	121.06	125.95
23	c	910	CLA	CMC-C2C-C1C	2.36	128.32	124.95
24	a	412	PHO	C4D-ND-C1D	-2.36	103.42	108.62
23	c	905	CLA	C3C-C4C-NC	2.36	113.00	110.15
23	b	618	CLA	CMA-C3A-C4A	-2.36	104.86	112.40
23	A	405	CLA	C4D-ND-C1D	-2.36	103.72	106.57
36	d	407	LHG	C11-C10-C9	-2.36	102.03	114.56
30	M	102	LMT	O6'-C6'-C5'	-2.36	103.16	111.37
23	d	403	CLA	CHB-C1B-NB	-2.36	120.70	124.70
23	B	612	CLA	CAA-CBA-CGA	-2.36	106.29	113.24
23	c	904	CLA	CBC-CAC-C3C	-2.36	105.23	112.37
23	A	410	CLA	C4D-CHA-C1A	-2.36	113.49	120.32
23	A	407	CLA	CED-O2D-CGD	2.36	121.61	116.00
23	c	909	CLA	CMC-C2C-C3C	2.36	132.76	126.04
23	B	613	CLA	C1C-C2C-C3C	-2.36	104.00	106.96
36	D	410	LHG	O7-C7-C8	2.36	116.56	111.54
23	B	616	CLA	CHC-C4B-NB	2.36	128.70	124.70
23	b	618	CLA	O2A-CGA-O1A	-2.35	117.33	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	601	HTG	C2'-C1'-S1	-2.35	105.33	112.64
23	a	411	CLA	OBD-CAD-C3D	-2.35	123.39	128.15
36	l	101	LHG	O8-C23-O10	-2.35	117.32	123.48
23	c	906	CLA	C3A-C4A-NA	2.36	113.66	110.81
23	c	906	CLA	C1C-C2C-C3C	-2.35	104.00	106.96
36	d	408	LHG	O8-C23-C24	2.35	119.10	111.90
23	c	907	CLA	C4B-CHC-C1C	-2.35	124.37	127.47
34	C	518	DGD	O1G-C1A-O1A	-2.35	117.33	123.48
23	A	405	CLA	CAA-C2A-C1A	-2.35	106.28	112.51
23	B	616	CLA	C2A-C1A-CHA	-2.35	119.59	123.87
30	b	625	LMT	O1'-C1'-C2'	-2.35	105.14	108.15
23	c	909	CLA	O2A-CGA-O1A	-2.35	117.33	123.48
23	B	610	CLA	C4C-C3C-C2C	-2.35	103.08	106.93
36	D	409	LHG	O8-C23-O10	-2.35	117.34	123.48
23	C	510	CLA	C4C-C3C-C2C	-2.35	103.08	106.93
23	c	913	CLA	CGD-CBD-CHA	-2.35	108.20	113.65
23	c	914	CLA	C4B-C3B-CAB	-2.35	122.42	127.18
23	B	602	CLA	CHC-C4B-NB	2.35	128.69	124.70
25	K	101	BCR	C39-C30-C25	-2.35	106.44	110.33
23	b	612	CLA	C1C-C2C-C3C	-2.35	104.01	106.96
24	A	408	PHO	CHD-C4C-C3C	-2.35	119.69	125.42
23	A	406	CLA	C16-C17-C18	-2.35	103.71	115.69
28	a	419	PL9	C10-C9-C11	2.35	118.95	115.39
38	H	101	RRX	C34-C9-C8	2.35	121.88	118.09
23	c	913	CLA	O2A-CGA-CBA	2.35	119.08	111.90
26	L	103	SQD	O9-S-O7	-2.34	105.30	113.45
24	A	409	PHO	CHD-C4C-C3C	-2.34	119.70	125.42
23	B	605	CLA	CHB-C1B-NB	-2.34	120.73	124.70
30	m	101	LMT	C3B-C4B-C5B	-2.34	105.97	110.17
23	a	411	CLA	C3A-C4A-NA	2.34	113.64	110.81
34	c	917	DGD	C3G-C2G-C1G	-2.34	106.49	111.86
23	a	411	CLA	O2A-CGA-CBA	2.34	119.06	111.90
23	a	410	CLA	O2A-C1-C2	-2.34	102.77	108.12
25	K	101	BCR	C37-C22-C21	-2.34	119.59	122.92
34	D	406	DGD	O1G-C1A-C2A	2.34	119.05	111.90
23	A	410	CLA	C3B-CAB-CBB	-2.34	121.11	125.95
23	b	606	CLA	C4B-NB-C1B	-2.34	104.87	107.12
23	C	504	CLA	C2D-C3D-CAD	2.34	144.47	134.94
23	B	616	CLA	CMB-C2B-C3B	2.33	129.56	125.16
23	B	604	CLA	O2A-C1-C2	-2.33	102.77	108.12
23	b	605	CLA	C2A-C1A-CHA	-2.33	119.62	123.87
26	a	401	SQD	C1-C2-C3	-2.33	105.47	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	418	SQD	O5-C5-C6	2.33	110.89	105.91
34	C	517	DGD	O1G-C1A-O1A	-2.33	117.38	123.48
23	C	506	CLA	C2B-C3B-CAB	2.33	132.10	127.33
34	C	516	DGD	CDB-CCB-CBB	-2.33	102.18	114.56
23	c	914	CLA	CED-O2D-CGD	2.33	121.55	116.00
23	c	904	CLA	C3C-C4C-NC	2.33	112.96	110.15
23	a	410	CLA	C3B-C4B-NB	2.33	112.22	109.21
23	C	512	CLA	C4B-C3B-CAB	-2.33	122.46	127.18
23	c	902	CLA	O2A-CGA-O1A	-2.33	117.39	123.48
23	b	606	CLA	C3A-C4A-NA	2.33	113.62	110.81
23	c	902	CLA	C2A-C1A-CHA	-2.33	119.64	123.87
25	T	101	BCR	C28-C27-C26	-2.32	109.99	113.81
25	d	404	BCR	C30-C25-C26	-2.33	119.22	122.59
23	C	512	CLA	C4A-NA-C1A	2.32	109.66	106.38
23	B	609	CLA	C11-C12-C13	-2.32	108.22	115.44
23	B	602	CLA	O2A-C1-C2	2.32	113.44	108.12
23	c	902	CLA	C4B-C3B-C2B	-2.32	104.65	107.04
23	b	616	CLA	C4A-NA-C1A	2.32	109.66	106.38
34	H	102	DGD	C3E-C4E-C5E	-2.32	106.00	110.17
23	c	912	CLA	CHB-C4A-NA	2.32	127.62	124.38
23	c	908	CLA	C5-C3-C2	-2.32	116.60	121.06
23	C	505	CLA	C4D-ND-C1D	2.32	109.37	106.57
23	b	606	CLA	O2A-CGA-O1A	-2.32	117.41	123.48
23	B	611	CLA	CAA-C2A-C3A	-2.32	107.51	113.32
23	c	914	CLA	C2B-C3B-CAB	2.32	132.07	127.33
38	H	101	RRX	C16-C17-C18	-2.32	123.94	127.29
23	d	402	CLA	C1C-NC-C4C	-2.32	103.14	106.26
23	C	511	CLA	CAC-C3C-C4C	2.32	128.33	124.85
36	D	408	LHG	C11-C10-C9	-2.32	102.27	114.56
34	c	919	DGD	C8B-C7B-C6B	-2.32	102.26	114.56
23	C	503	CLA	C2A-C1A-NA	2.32	114.30	111.33
23	c	909	CLA	C2A-C1A-CHA	-2.32	119.65	123.87
23	b	606	CLA	C7-C6-C5	-2.32	106.20	112.97
23	a	414	CLA	C2D-C3D-CAD	2.32	144.38	134.94
30	M	101	LMT	C2'-C3'-C4'	2.32	114.61	109.59
23	C	513	CLA	O2A-CGA-O1A	-2.31	117.44	123.48
23	b	608	CLA	C2D-C3D-CAD	2.31	144.37	134.94
23	b	609	CLA	C4-C3-C5	2.31	118.90	115.39
25	d	404	BCR	C34-C9-C8	2.31	121.83	118.09
34	c	917	DGD	O2G-C1B-C2B	2.31	116.47	111.54
27	A	413	LMG	O8-C28-C29	2.31	118.97	111.90
30	M	101	LMT	O2'-C2'-C3'	-2.31	105.20	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	BCR	C23-C24-C25	-2.31	120.42	127.23
25	c	916	BCR	C35-C13-C12	2.31	121.82	118.09
30	t	102	LMT	C1-O1'-C1'	-2.31	109.84	113.91
23	a	414	CLA	C3A-C4A-CHB	-2.31	119.53	124.33
23	c	903	CLA	O2A-CGA-O1A	-2.31	117.44	123.48
24	a	412	PHO	CAA-C2A-C3A	-2.31	107.54	113.32
26	a	401	SQD	O48-C23-O10	-2.31	117.45	123.48
25	K	101	BCR	C7-C8-C9	-2.31	122.77	126.22
23	D	402	CLA	C2B-C1B-NB	2.31	111.04	109.50
23	c	910	CLA	C4C-C3C-C2C	-2.31	103.15	106.93
23	c	904	CLA	CED-O2D-CGD	2.31	121.49	116.00
23	b	606	CLA	C2D-C3D-CAD	2.31	144.34	134.94
23	D	402	CLA	CMB-C2B-C1B	-2.30	124.92	128.46
34	c	918	DGD	O2G-C1B-O1B	-2.30	117.52	123.66
23	a	409	CLA	C1-C2-C3	-2.30	122.24	126.23
23	c	904	CLA	O2A-CGA-CBA	2.30	118.94	111.90
23	b	610	CLA	O2D-CGD-CBD	2.30	115.99	111.34
33	b	626	HTG	C1'-S1-C1	2.30	103.53	100.19
34	C	518	DGD	O2G-C1B-O1B	-2.30	117.53	123.66
23	B	613	CLA	C2B-C1B-CHB	-2.30	121.64	126.00
26	D	407	SQD	O48-C23-O10	-2.30	117.48	123.48
23	A	405	CLA	CHB-C4A-NA	2.30	127.58	124.38
26	f	102	SQD	O6-C44-C45	2.30	114.83	108.80
23	B	606	CLA	O2D-CGD-O1D	-2.29	119.19	123.79
28	d	405	PL9	C11-C9-C8	-2.29	116.65	121.06
23	a	409	CLA	O2A-CGA-CBA	2.29	118.92	111.90
23	a	411	CLA	C3D-CAD-CBD	2.29	110.84	107.60
23	B	607	CLA	O1D-CGD-CBD	-2.29	119.77	124.45
23	B	611	CLA	C3C-C4C-NC	2.29	112.91	110.15
23	b	612	CLA	C4B-C3B-CAB	-2.29	122.54	127.18
23	B	603	CLA	C14-C13-C12	-2.29	102.10	111.05
25	B	619	BCR	C15-C16-C17	-2.29	118.40	123.45
23	B	617	CLA	C1C-C2C-C3C	-2.29	104.08	106.96
23	c	903	CLA	C2B-C3B-CAB	2.29	132.01	127.33
23	B	611	CLA	C4C-C3C-C2C	-2.29	103.18	106.93
23	C	509	CLA	CHC-C1C-C2C	-2.29	120.36	126.51
34	h	102	DGD	C6D-C5D-C4D	2.29	117.17	111.98
23	B	614	CLA	O2A-CGA-O1A	-2.29	117.49	123.48
23	B	602	CLA	C2B-C1B-CHB	-2.29	121.66	126.00
27	c	920	LMG	O1-C7-C8	-2.29	105.55	110.99
23	A	405	CLA	C2B-C1B-CHB	-2.29	121.67	126.00
23	C	501	CLA	C1-C2-C3	-2.29	122.26	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C2B-C3B-CAB	2.28	132.00	127.33
23	C	513	CLA	C2A-C1A-CHA	-2.28	119.72	123.87
23	B	602	CLA	OBD-CAD-C3D	-2.28	123.54	128.15
23	b	618	CLA	C11-C10-C8	-2.28	108.35	115.44
34	c	919	DGD	O1G-C1G-C2G	-2.28	102.81	108.80
23	b	613	CLA	C4B-C3B-C2B	-2.28	104.70	107.04
23	C	505	CLA	C2D-C1D-ND	2.28	112.16	109.56
23	b	610	CLA	CBC-CAC-C3C	-2.28	105.46	112.37
23	C	505	CLA	C2D-C3D-CAD	2.28	144.23	134.94
36	D	409	LHG	C13-C12-C11	-2.28	102.46	114.56
23	c	906	CLA	C4A-NA-C1A	2.28	109.59	106.38
23	c	905	CLA	CMD-C2D-C3D	2.28	129.45	125.16
23	a	411	CLA	C2D-C3D-CAD	2.28	144.23	134.94
26	a	416	SQD	O48-C46-C45	-2.28	102.81	108.80
25	b	622	BCR	C23-C22-C21	-2.28	115.47	118.98
23	B	614	CLA	C4C-C3C-C2C	-2.28	103.20	106.93
23	B	611	CLA	CAC-C3C-C4C	2.28	128.27	124.85
25	b	620	BCR	C16-C17-C18	-2.27	124.00	127.29
24	A	409	PHO	C4A-NA-C1A	2.28	111.41	108.42
23	B	608	CLA	C7-C6-C5	-2.28	106.33	112.97
34	C	516	DGD	C6D-O5D-C1E	-2.28	109.23	113.80
30	t	102	LMT	O5'-C5'-C4'	-2.27	106.93	110.42
23	c	912	CLA	C5-C3-C2	-2.27	116.69	121.06
34	C	516	DGD	C1G-O1G-C1A	2.27	123.48	116.99
25	D	404	BCR	C21-C20-C19	-2.27	115.61	123.23
27	b	623	LMG	C1-O6-C5	-2.27	109.33	113.73
23	d	403	CLA	CAC-C3C-C4C	2.27	128.26	124.85
30	b	625	LMT	C1-O1'-C1'	2.27	117.92	113.91
25	B	619	BCR	C30-C25-C26	-2.27	119.30	122.59
36	l	101	LHG	O3-P-O5	-2.27	100.47	109.37
23	b	609	CLA	C1-O2A-CGA	2.27	123.61	117.00
27	d	410	LMG	O1-C7-C8	-2.27	105.59	110.99
23	D	403	CLA	C2D-C3D-CAD	2.27	144.20	134.94
23	B	609	CLA	C3B-CAB-CBB	-2.27	121.25	125.95
34	D	406	DGD	O6D-C5D-C4D	2.27	113.95	109.73
23	A	406	CLA	CMC-C2C-C1C	2.27	128.18	124.95
26	L	103	SQD	C5-C6-S	2.27	117.57	114.40
23	D	402	CLA	OBD-CAD-CBD	2.27	129.36	125.94
25	k	101	BCR	C1-C6-C7	2.27	121.97	115.69
27	d	410	LMG	O2-C2-C1	-2.27	105.11	110.03
23	b	610	CLA	C4B-C3B-CAB	-2.27	122.59	127.18
27	D	411	LMG	O8-C28-C29	2.27	118.83	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	415	BCR	C35-C13-C12	2.26	121.75	118.09
25	C	514	BCR	C37-C22-C23	2.26	121.75	118.09
26	D	407	SQD	O5-C1-O6	2.26	115.31	109.93
26	D	407	SQD	O4-C4-C3	-2.26	105.30	110.36
24	a	413	PHO	CHD-C4C-NC	-2.26	124.64	128.68
23	c	904	CLA	O2D-CGD-O1D	-2.26	119.25	123.79
25	C	514	BCR	C40-C30-C25	-2.26	106.58	110.33
25	b	622	BCR	C40-C30-C25	-2.26	106.58	110.33
23	b	610	CLA	C1-C2-C3	-2.26	122.30	126.23
25	D	404	BCR	C38-C26-C27	2.26	117.68	113.39
23	B	603	CLA	C4C-C3C-C2C	-2.26	103.23	106.93
27	B	622	LMG	C9-O8-C28	-2.26	110.54	116.99
28	a	419	PL9	C26-C24-C23	-2.26	116.72	121.06
23	b	615	CLA	CED-O2D-CGD	2.26	121.38	116.00
23	b	617	CLA	C2B-C3B-CAB	2.26	131.94	127.33
23	C	512	CLA	CHC-C4B-NB	2.26	128.53	124.70
23	c	902	CLA	C4B-NB-C1B	-2.26	104.94	107.12
23	a	414	CLA	O2A-CGA-CBA	2.26	118.81	111.90
23	b	604	CLA	C2D-C3D-CAD	2.26	144.15	134.94
23	C	510	CLA	C3B-CAB-CBB	-2.26	121.28	125.95
23	B	614	CLA	C3B-C4B-NB	2.26	112.13	109.21
36	L	101	LHG	C34-C33-C32	-2.25	102.59	114.56
23	A	410	CLA	C6-C5-C3	2.26	117.77	112.62
23	B	608	CLA	C3A-C2A-C1A	-2.26	98.04	101.70
23	c	906	CLA	O2A-CGA-O1A	-2.26	117.58	123.48
23	b	614	CLA	CBA-CAA-C2A	-2.26	108.43	113.95
30	a	402	LMT	O5B-C5B-C6B	2.25	111.95	106.34
25	b	621	BCR	C8-C9-C10	-2.25	115.51	118.98
23	C	504	CLA	C7-C6-C5	-2.25	106.39	112.97
23	b	619	CLA	CBC-CAC-C3C	-2.25	105.55	112.37
23	b	611	CLA	C3B-CAB-CBB	-2.25	121.29	125.95
23	D	403	CLA	CBC-CAC-C3C	-2.25	105.55	112.37
28	D	405	PL9	C11-C9-C8	-2.25	116.74	121.06
26	D	407	SQD	O6-C44-C45	2.25	116.33	110.99
23	B	604	CLA	C1C-NC-C4C	-2.25	103.23	106.26
23	B	602	CLA	OBD-CAD-CBD	2.25	129.33	125.94
23	a	414	CLA	C4C-C3C-C2C	-2.25	103.25	106.93
23	A	405	CLA	CHC-C1C-C2C	-2.24	120.48	126.51
23	A	405	CLA	C4C-C3C-C2C	-2.24	103.25	106.93
23	b	611	CLA	CMC-C2C-C1C	2.24	128.15	124.95
25	b	620	BCR	C21-C20-C19	-2.24	115.70	123.23
28	a	419	PL9	C45-C44-C43	-2.24	119.05	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C12-C11-C10	-2.24	101.94	113.00
23	b	609	CLA	O2A-CGA-CBA	2.24	118.76	111.90
26	A	418	SQD	C44-O6-C1	2.24	118.30	113.80
23	c	903	CLA	O2A-CGA-CBA	2.24	118.76	111.90
28	a	419	PL9	C27-C28-C29	-2.24	122.96	127.81
23	c	911	CLA	C2A-C1A-CHA	-2.24	119.80	123.87
23	a	409	CLA	CMC-C2C-C3C	2.24	132.42	126.04
23	b	619	CLA	C1-O2A-CGA	2.24	123.51	117.00
33	B	630	HTG	O2-C2-C3	2.24	115.36	110.36
26	A	418	SQD	O8-S-O9	-2.24	106.71	111.69
37	v	201	HEM	CMA-C3A-C4A	-2.24	125.03	128.46
25	b	620	BCR	C39-C30-C29	-2.24	99.90	108.78
25	K	101	BCR	C10-C11-C12	-2.23	115.74	123.23
23	a	409	CLA	C3C-C4C-NC	2.23	112.84	110.15
23	c	902	CLA	CMB-C2B-C1B	2.23	131.90	128.46
23	c	907	CLA	C4B-NB-C1B	-2.23	104.97	107.12
23	C	510	CLA	C3A-C4A-CHB	-2.23	119.68	124.33
23	b	609	CLA	CBC-CAC-C3C	-2.23	105.61	112.37
23	c	905	CLA	O2D-CGD-O1D	-2.23	119.31	123.79
25	K	101	BCR	C38-C26-C27	2.23	117.62	113.39
38	h	101	RRX	C11-C10-C9	-2.23	124.06	127.29
23	C	502	CLA	C3B-C4B-NB	2.23	112.09	109.21
25	C	514	BCR	C2-C1-C6	2.23	113.93	110.37
23	c	907	CLA	C2A-C1A-NA	2.23	114.19	111.33
23	D	403	CLA	C4-C3-C5	2.23	118.78	115.39
23	a	409	CLA	C2B-C1B-CHB	-2.23	121.77	126.00
23	c	913	CLA	CMB-C2B-C1B	2.23	131.89	128.46
23	d	402	CLA	CMB-C2B-C3B	2.23	129.36	125.16
23	B	615	CLA	CMD-C2D-C1D	2.23	130.56	126.16
23	B	607	CLA	C4B-C3B-CAB	-2.23	122.66	127.18
23	c	913	CLA	CBC-CAC-C3C	-2.23	105.62	112.37
33	B	625	HTG	O2-C2-C3	-2.23	105.38	110.36
30	M	102	LMT	O2B-C2B-C1B	-2.23	105.20	110.03
23	a	409	CLA	CHC-C4B-NB	2.23	128.48	124.70
23	a	414	CLA	OBD-CAD-C3D	-2.23	123.65	128.15
23	C	505	CLA	OBD-CAD-C3D	-2.22	123.66	128.15
23	c	906	CLA	C11-C12-C13	-2.22	108.52	115.44
23	B	609	CLA	C2D-C3D-CAD	2.22	144.00	134.94
23	c	908	CLA	C2D-C3D-CAD	2.22	144.00	134.94
25	K	102	BCR	C37-C22-C21	-2.22	119.75	122.92
26	L	103	SQD	O48-C23-C24	2.22	118.70	111.90
23	C	508	CLA	C4A-NA-C1A	2.22	109.51	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	911	CLA	C3A-C4A-NA	2.22	113.50	110.81
23	B	602	CLA	C2A-C1A-CHA	-2.22	119.83	123.87
23	b	616	CLA	CHC-C4B-NB	2.22	128.47	124.70
28	A	414	PL9	C10-C9-C11	2.22	118.76	115.39
23	B	615	CLA	C2A-C1A-CHA	-2.22	119.83	123.87
34	c	919	DGD	C4E-C3E-C2E	2.22	114.89	110.80
34	C	516	DGD	O6E-C1E-C2E	-2.22	105.76	110.30
30	J	102	LMT	C1'-C2'-C3'	2.22	114.28	109.99
36	l	101	LHG	O4-P-O5	2.22	124.41	112.14
23	b	607	CLA	CMD-C2D-C1D	2.22	130.54	126.16
23	c	905	CLA	CMD-C2D-C1D	2.22	130.54	126.16
26	f	102	SQD	O8-S-O9	-2.21	106.76	111.69
23	d	403	CLA	C2D-C3D-CAD	2.21	143.95	134.94
23	C	503	CLA	C5-C3-C2	-2.21	116.81	121.06
27	C	519	LMG	C9-C8-C7	-2.21	106.78	111.86
23	b	617	CLA	C4B-NB-C1B	-2.21	104.99	107.12
23	b	612	CLA	C4-C3-C5	2.21	118.74	115.39
27	c	921	LMG	O6-C1-C2	-2.21	105.79	110.30
23	D	402	CLA	C3B-C2B-C1B	-2.21	104.25	106.69
23	b	613	CLA	O2A-CGA-CBA	2.21	118.65	111.90
23	c	904	CLA	C7-C6-C5	-2.21	106.53	112.97
24	A	409	PHO	C1D-CHD-C4C	-2.20	122.00	126.23
23	c	906	CLA	C2D-C3D-CAD	2.20	143.93	134.94
23	C	507	CLA	CHB-C4A-NA	2.20	127.45	124.38
23	A	406	CLA	O2A-C1-C2	-2.20	103.08	108.12
30	M	102	LMT	O4'-C4B-C3B	2.20	115.27	110.36
23	b	617	CLA	C2A-C1A-CHA	-2.20	119.87	123.87
38	h	101	RRX	C20-C21-C22	-2.20	124.11	127.29
23	c	909	CLA	CAC-C3C-C2C	2.20	131.47	127.50
34	H	102	DGD	O2G-C1B-C2B	2.20	116.23	111.54
23	b	610	CLA	C2D-C3D-CAD	2.20	143.90	134.94
23	b	608	CLA	C1-C2-C3	-2.20	122.42	126.23
23	C	510	CLA	C2D-C3D-CAD	2.20	143.90	134.94
25	T	101	BCR	C19-C18-C17	-2.20	115.60	118.98
38	h	101	RRX	C24-C23-C22	-2.20	122.93	126.22
36	d	407	LHG	O8-C6-C5	-2.20	103.03	108.80
34	C	518	DGD	C3D-C4D-C5D	-2.19	106.23	110.17
23	B	603	CLA	C3B-C4B-NB	2.19	112.05	109.21
23	B	616	CLA	C4B-C3B-C2B	-2.19	104.78	107.04
23	c	911	CLA	C1-C2-C3	-2.19	122.42	126.23
23	C	502	CLA	C16-C17-C18	-2.19	104.48	115.69
23	b	607	CLA	C7-C6-C5	-2.19	106.57	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C2D-C3D-CAD	2.19	143.88	134.94
23	c	909	CLA	C3C-C4C-NC	2.19	112.79	110.15
23	B	617	CLA	C2D-C3D-CAD	2.19	143.88	134.94
23	D	402	CLA	C3C-C4C-NC	2.19	112.79	110.15
23	C	506	CLA	O1D-CGD-CBD	-2.19	119.97	124.45
33	b	602	HTG	C2-C1-S1	2.19	113.44	110.97
24	A	408	PHO	C7-C6-C5	-2.19	106.57	112.97
23	C	512	CLA	C4B-CHC-C1C	-2.19	124.59	127.47
23	c	902	CLA	O2A-CGA-CBA	2.19	118.60	111.90
25	D	404	BCR	C40-C30-C39	2.19	115.86	108.47
23	b	604	CLA	CED-O2D-CGD	2.19	121.22	116.00
33	b	602	HTG	C1-O5-C5	2.19	117.11	112.78
23	B	604	CLA	CAA-C2A-C1A	-2.19	106.72	112.51
33	B	625	HTG	O4-C4-C5	2.19	115.05	109.25
23	d	402	CLA	C3D-CAD-CBD	2.19	110.69	107.60
23	B	602	CLA	C4D-C3D-CAD	2.19	110.74	108.05
38	h	101	RRX	C33-C5-C6	-2.18	122.03	124.50
23	B	613	CLA	C4C-C3C-C2C	-2.18	103.35	106.93
23	b	609	CLA	CMD-C2D-C1D	2.18	130.48	126.16
26	a	416	SQD	O48-C23-O10	-2.19	117.77	123.48
23	c	910	CLA	CHB-C1B-NB	-2.18	121.00	124.70
25	b	621	BCR	C35-C13-C14	-2.18	119.81	122.92
25	b	621	BCR	C16-C15-C14	-2.18	118.64	123.45
23	b	619	CLA	O2A-CGA-O1A	-2.18	117.77	123.48
25	K	101	BCR	C29-C28-C27	-2.18	105.84	111.46
23	b	613	CLA	C1D-CHD-C4C	-2.18	119.22	122.60
23	C	502	CLA	CBA-CAA-C2A	-2.18	108.61	113.95
30	c	922	LMT	O3B-C3B-C4B	2.18	115.23	110.36
37	F	101	HEM	CMA-C3A-C2A	2.18	129.06	124.94
23	B	606	CLA	C3B-CAB-CBB	-2.18	121.44	125.95
23	B	612	CLA	C4-C3-C5	2.18	118.70	115.39
28	A	414	PL9	C15-C14-C16	2.18	118.70	115.39
26	a	416	SQD	O48-C23-C24	2.18	118.57	111.90
23	C	509	CLA	C2D-C3D-CAD	2.18	143.83	134.94
23	C	512	CLA	C1D-CHD-C4C	-2.18	119.22	122.60
23	A	406	CLA	C11-C10-C8	-2.18	108.67	115.44
23	d	403	CLA	C2B-C3B-CAB	2.18	131.78	127.33
25	k	101	BCR	C33-C5-C6	-2.18	122.04	124.50
23	c	908	CLA	C4C-C3C-C2C	-2.18	103.36	106.93
23	c	907	CLA	O2A-CGA-CBA	2.18	118.56	111.90
34	c	917	DGD	CDB-CCB-CBB	-2.17	103.02	114.56
23	b	618	CLA	OBD-CAD-CBD	2.17	129.22	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	618	CLA	C5-C3-C2	-2.17	116.88	121.06
25	K	101	BCR	C4-C5-C6	2.17	125.73	122.86
26	L	103	SQD	C6-C5-C4	2.17	116.45	111.86
36	a	417	LHG	C6-O8-C23	2.17	123.20	116.99
27	c	920	LMG	C3-C4-C5	2.17	114.07	110.17
23	c	911	CLA	C4C-C3C-C2C	-2.17	103.37	106.93
25	B	619	BCR	C7-C8-C9	-2.17	122.96	126.22
27	d	410	LMG	O8-C9-C8	-2.17	103.08	108.80
24	A	408	PHO	CAA-C2A-C1A	-2.17	107.03	112.78
23	c	905	CLA	CMB-C2B-C3B	2.17	129.25	125.16
23	A	406	CLA	C3B-C4B-NB	2.17	112.02	109.21
25	b	620	BCR	C40-C30-C25	-2.17	106.73	110.33
23	b	608	CLA	CBA-CAA-C2A	-2.17	108.64	113.95
26	A	412	SQD	C9-C8-C7	-2.17	105.09	113.51
23	c	910	CLA	O2A-CGA-O1A	-2.17	117.80	123.48
27	b	623	LMG	O1-C1-C2	2.17	110.93	108.15
23	B	610	CLA	CED-O2D-CGD	2.17	121.17	116.00
23	B	612	CLA	C4A-NA-C1A	2.17	109.44	106.38
26	L	103	SQD	C1-O5-C5	-2.17	109.54	113.73
23	B	611	CLA	C4A-NA-C1A	2.17	109.44	106.38
23	C	501	CLA	CMC-C2C-C1C	2.17	128.04	124.95
25	c	916	BCR	C19-C18-C17	-2.17	115.64	118.98
24	A	408	PHO	C4D-C3D-C2D	2.17	109.61	107.01
23	B	614	CLA	C4B-C3B-C2B	-2.17	104.81	107.04
23	C	513	CLA	OBD-CAD-C3D	-2.16	123.78	128.15
24	A	408	PHO	C1D-CHD-C4C	-2.16	122.08	126.23
23	C	502	CLA	C2D-C3D-CAD	2.16	143.76	134.94
23	A	406	CLA	C2A-C1A-CHA	-2.16	119.94	123.87
25	B	618	BCR	C24-C25-C26	2.16	126.79	121.59
33	B	624	HTG	O5-C5-C6	2.16	111.73	106.34
23	C	510	CLA	C3C-C4C-NC	2.16	112.76	110.15
30	C	520	LMT	C3'-C4'-C5'	-2.16	106.03	110.86
23	c	908	CLA	O2A-CGA-O1A	-2.16	117.83	123.48
25	T	101	BCR	C21-C20-C19	-2.16	115.98	123.23
36	d	409	LHG	O8-C23-C24	2.16	118.51	111.90
30	m	101	LMT	C6'-C5'-C4'	2.16	119.46	113.27
23	c	913	CLA	CMD-C2D-C3D	2.16	129.23	125.16
23	C	506	CLA	O2A-CGA-O1A	-2.16	117.83	123.48
23	D	402	CLA	C4C-C3C-C2C	-2.16	103.39	106.93
23	c	911	CLA	O2D-CGD-O1D	-2.16	119.46	123.79
36	d	409	LHG	O8-C23-O10	-2.16	117.84	123.48
23	C	503	CLA	CMC-C2C-C1C	2.16	128.03	124.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	410	CLA	O2D-CGD-O1D	-2.16	119.46	123.79
30	a	402	LMT	O2'-C2'-C3'	-2.16	105.53	110.36
23	b	619	CLA	C2B-C1B-CHB	-2.16	121.91	126.00
23	A	407	CLA	CGD-CBD-CAD	-2.16	103.54	110.79
23	c	909	CLA	O2D-CGD-CBD	2.16	115.70	111.34
24	A	408	PHO	C16-C17-C18	-2.16	104.66	115.69
23	c	906	CLA	C4C-C3C-C2C	-2.16	103.39	106.93
23	B	615	CLA	C2B-C1B-CHB	-2.16	121.91	126.00
36	d	407	LHG	O7-C7-O9	-2.16	117.91	123.66
28	A	414	PL9	C12-C13-C14	-2.16	123.15	127.81
23	b	609	CLA	CGD-CBD-CHA	-2.16	108.65	113.65
27	A	413	LMG	O2-C2-C3	-2.15	105.55	110.36
23	C	508	CLA	C4C-C3C-C2C	-2.15	103.40	106.93
23	b	608	CLA	C5-C3-C2	-2.15	116.92	121.06
23	c	907	CLA	C3B-CAB-CBB	-2.15	121.49	125.95
23	c	910	CLA	O2A-CGA-CBA	2.16	118.50	111.90
25	d	404	BCR	C37-C22-C21	-2.15	119.85	122.92
23	B	614	CLA	C3C-C4C-NC	2.15	112.75	110.15
25	B	618	BCR	C34-C9-C10	-2.15	119.85	122.92
23	c	908	CLA	O1D-CGD-CBD	-2.15	120.05	124.45
23	c	908	CLA	C11-C12-C13	-2.15	108.74	115.44
23	c	914	CLA	CAA-CBA-CGA	-2.15	106.91	113.24
25	C	514	BCR	C29-C30-C25	2.15	113.80	110.37
30	b	624	LMT	C1'-O5'-C5'	2.15	117.89	113.73
23	c	914	CLA	C2D-C3D-CAD	2.15	143.70	134.94
23	D	403	CLA	CMB-C2B-C3B	2.15	129.21	125.16
25	K	102	BCR	C34-C9-C8	2.15	121.56	118.09
23	B	613	CLA	O2A-CGA-CBA	2.15	118.47	111.90
23	B	615	CLA	C2A-C1A-NA	2.15	114.08	111.33
23	b	610	CLA	C4D-ND-C1D	2.15	109.16	106.57
23	d	402	CLA	C2A-C1A-CHA	-2.14	119.97	123.87
23	B	606	CLA	C2D-C3D-CAD	2.14	143.68	134.94
25	K	102	BCR	C34-C9-C10	-2.14	119.86	122.92
25	b	621	BCR	C11-C12-C13	-2.14	120.23	126.37
23	B	612	CLA	O2A-CGA-O1A	-2.14	117.88	123.48
34	H	102	DGD	C3D-C4D-C5D	-2.14	106.33	110.17
27	B	622	LMG	O4-C4-C3	-2.14	105.57	110.36
23	c	903	CLA	C4C-C3C-C2C	-2.14	103.42	106.93
23	c	908	CLA	CAC-C3C-C4C	2.14	128.06	124.85
25	B	619	BCR	C37-C22-C23	2.14	121.55	118.09
23	B	615	CLA	C4A-NA-C1A	2.14	109.40	106.38
23	A	405	CLA	C3A-C4A-CHB	-2.14	119.88	124.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	912	CLA	O2A-CGA-O1A	-2.14	117.89	123.48
23	b	613	CLA	CMC-C2C-C1C	2.14	128.00	124.95
23	A	407	CLA	CMA-C3A-C4A	-2.14	105.56	112.40
23	b	610	CLA	C7-C6-C5	-2.14	106.72	112.97
23	D	402	CLA	C2B-C3B-CAB	2.14	131.70	127.33
23	c	908	CLA	CMC-C2C-C1C	2.14	128.00	124.95
23	B	615	CLA	C4B-C3B-CAB	-2.14	122.85	127.18
23	d	402	CLA	CHC-C1C-C2C	-2.13	120.78	126.51
28	D	405	PL9	C51-C49-C50	2.13	119.99	114.62
23	C	505	CLA	C3B-C4B-NB	2.13	111.97	109.21
27	d	410	LMG	C9-C8-C7	-2.13	106.96	111.86
23	c	905	CLA	C2A-C1A-CHA	-2.13	119.99	123.87
23	B	608	CLA	CHB-C1B-NB	-2.13	121.08	124.70
30	z	101	LMT	O1B-C4'-C3'	2.13	112.57	107.17
23	C	506	CLA	C4A-NA-C1A	2.13	109.38	106.38
25	C	515	BCR	C40-C30-C25	-2.13	106.80	110.33
23	B	607	CLA	C2D-C3D-CAD	2.13	143.63	134.94
26	B	621	SQD	O8-S-O9	-2.13	106.95	111.69
23	b	617	CLA	C3A-C4A-CHB	-2.13	119.90	124.33
37	f	101	HEM	C3A-C4A-NA	-2.13	108.08	109.50
23	B	608	CLA	O2D-CGD-CBD	2.13	115.64	111.34
23	C	504	CLA	CMD-C2D-C1D	2.13	130.37	126.16
23	b	618	CLA	OBD-CAD-C3D	-2.13	123.85	128.15
23	D	402	CLA	C5-C3-C2	-2.13	116.97	121.06
23	b	618	CLA	O2A-C1-C2	2.13	112.99	108.12
23	C	513	CLA	CAA-C2A-C1A	-2.13	106.88	112.51
23	B	604	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
23	B	604	CLA	CHC-C1C-NC	-2.13	119.19	123.42
23	a	409	CLA	C3A-C4A-NA	2.13	113.38	110.81
23	C	501	CLA	C1-O2A-CGA	2.13	123.18	117.00
23	C	510	CLA	O2D-CGD-CBD	2.12	115.63	111.34
23	B	616	CLA	C5-C3-C2	-2.12	116.98	121.06
23	a	409	CLA	C3B-CAB-CBB	-2.12	121.56	125.95
26	A	412	SQD	O5-C1-C2	-2.12	105.96	110.30
30	C	520	LMT	O3B-C3B-C2B	-2.12	105.61	110.36
28	D	405	PL9	C46-C47-C48	-2.12	105.61	111.64
25	a	415	BCR	C8-C7-C6	-2.12	120.98	127.23
23	C	508	CLA	C1D-CHD-C4C	2.12	125.89	122.60
28	d	405	PL9	C7-C8-C9	-2.12	123.17	126.76
23	B	605	CLA	CMD-C2D-C1D	2.12	130.35	126.16
23	b	609	CLA	CMD-C2D-C3D	2.12	129.16	125.16
23	B	612	CLA	CAC-C3C-C4C	2.12	128.03	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C16-C15-C13	2.12	122.03	115.44
23	B	617	CLA	C3A-C4A-NA	2.12	113.37	110.81
23	B	615	CLA	C2D-C3D-CAD	2.12	143.58	134.94
23	A	406	CLA	C2D-C3D-CAD	2.12	143.57	134.94
36	E	101	LHG	C6-O8-C23	2.12	123.04	116.99
23	c	905	CLA	C2B-C3B-CAB	2.12	131.66	127.33
23	A	406	CLA	C4D-ND-C1D	2.11	109.12	106.57
25	k	101	BCR	C15-C16-C17	-2.11	118.79	123.45
37	V	201	HEM	CMA-C3A-C4A	-2.12	125.21	128.46
23	c	905	CLA	O2A-C1-C2	-2.12	103.28	108.12
23	d	402	CLA	C2A-C1A-NA	2.11	114.04	111.33
26	L	103	SQD	O5-C5-C6	2.11	110.42	105.91
23	B	609	CLA	C11-C10-C8	-2.11	108.88	115.44
25	D	404	BCR	C32-C1-C2	-2.11	100.39	108.78
23	c	903	CLA	C4B-C3B-CAB	-2.11	122.90	127.18
23	c	903	CLA	C16-C17-C18	-2.11	104.91	115.69
36	L	101	LHG	C13-C12-C11	-2.11	103.37	114.56
24	a	412	PHO	C7-C6-C5	-2.11	106.81	112.97
23	C	503	CLA	OBD-CAD-C3D	-2.11	123.89	128.15
23	B	605	CLA	C3B-C4B-NB	2.11	111.94	109.21
23	B	608	CLA	CAA-C2A-C3A	-2.11	108.04	113.32
23	c	902	CLA	C2D-C3D-CAD	2.11	143.54	134.94
23	b	609	CLA	C4B-NB-C1B	-2.11	105.09	107.12
25	D	404	BCR	C39-C30-C25	-2.11	106.84	110.33
23	c	912	CLA	C4D-C3D-CAD	2.11	110.64	108.05
23	c	904	CLA	OBD-CAD-CBD	2.11	129.12	125.94
37	v	201	HEM	C2A-C1A-NA	-2.11	106.81	109.73
23	b	608	CLA	CAC-C3C-C2C	-2.10	123.71	127.50
23	b	605	CLA	CED-O2D-CGD	2.11	121.01	116.00
26	A	412	SQD	O9-S-O7	-2.11	106.13	113.45
37	V	201	HEM	CMB-C2B-C3B	2.11	131.04	126.21
23	B	613	CLA	C4A-NA-C1A	2.10	109.34	106.38
25	B	620	BCR	C10-C11-C12	-2.10	116.17	123.23
34	c	918	DGD	O4E-C4E-C3E	-2.10	105.66	110.36
38	h	101	RRX	C34-C9-C8	2.10	121.49	118.09
23	b	616	CLA	CMD-C2D-C3D	2.10	129.12	125.16
23	D	402	CLA	CAA-C2A-C3A	-2.10	108.06	113.32
28	a	419	PL9	C16-C14-C13	-2.10	117.02	121.06
23	b	609	CLA	CHC-C1C-C2C	-2.10	120.87	126.51
23	B	611	CLA	C2A-C1A-CHA	-2.10	120.05	123.87
25	c	915	BCR	C35-C13-C12	2.10	121.48	118.09
28	D	405	PL9	C27-C26-C24	-2.10	105.81	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	z	101	LMT	O1B-C1B-C2B	2.10	113.14	108.11
23	c	910	CLA	C4B-C3B-CAB	-2.10	122.93	127.18
23	B	610	CLA	CBA-CAA-C2A	-2.10	108.81	113.95
23	C	506	CLA	O2A-CGA-CBA	2.10	118.32	111.90
23	a	411	CLA	O2A-CGA-O1A	-2.10	118.00	123.48
24	a	412	PHO	C2B-C1B-NB	2.10	113.58	106.15
24	A	409	PHO	C4C-NC-C1C	-2.10	102.35	106.52
23	C	507	CLA	C3C-C4C-NC	2.10	112.68	110.15
25	d	404	BCR	C32-C1-C2	-2.10	100.44	108.78
23	a	410	CLA	CGD-CBD-CAD	-2.10	103.75	110.79
23	C	504	CLA	C4A-NA-C1A	2.10	109.33	106.38
25	c	916	BCR	C7-C8-C9	-2.09	123.08	126.22
34	C	517	DGD	CGA-CFA-CEA	-2.09	106.95	112.94
23	B	614	CLA	C2D-C3D-CAD	2.09	143.47	134.94
25	b	620	BCR	C15-C16-C17	-2.09	118.84	123.45
23	b	611	CLA	C6-C7-C8	-2.09	108.94	115.44
23	B	604	CLA	C4A-NA-C1A	2.09	109.33	106.38
24	a	413	PHO	C3D-CAD-CBD	2.09	110.55	107.60
26	A	412	SQD	O48-C23-C24	2.09	118.30	111.90
23	a	410	CLA	O2D-CGD-O1D	-2.09	119.59	123.79
23	a	410	CLA	C4-C3-C5	2.09	118.56	115.39
23	D	403	CLA	CMD-C2D-C3D	2.09	129.10	125.16
30	t	102	LMT	O2'-C2'-C3'	-2.09	105.69	110.36
38	H	101	RRX	C23-C24-C25	-2.09	121.07	127.23
28	d	405	PL9	C3-C4-C5	2.09	121.60	118.69
23	b	616	CLA	C2B-C1B-CHB	-2.09	122.04	126.00
34	D	406	DGD	C3D-C4D-C5D	2.09	113.92	110.17
36	D	409	LHG	O7-C7-O9	-2.09	118.09	123.66
30	M	102	LMT	C3B-C4B-C5B	-2.09	106.43	110.17
25	k	101	BCR	C20-C21-C22	-2.08	124.28	127.29
25	k	101	BCR	C29-C30-C25	2.08	113.69	110.37
23	C	508	CLA	CHB-C4A-NA	2.08	127.29	124.38
23	b	612	CLA	C3A-C4A-NA	2.08	113.33	110.81
23	B	603	CLA	C3C-C4C-NC	2.08	112.66	110.15
23	D	402	CLA	C3A-C2A-C1A	-2.08	98.32	101.70
30	a	402	LMT	C8-C7-C6	-2.08	103.50	114.56
25	K	102	BCR	C37-C22-C23	2.08	121.45	118.09
23	b	606	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
25	k	102	BCR	C28-C27-C26	-2.08	110.39	113.81
23	b	608	CLA	C14-C13-C12	-2.08	102.91	111.05
23	C	502	CLA	C4B-C3B-CAB	-2.08	122.96	127.18
23	c	903	CLA	C2D-C3D-CAD	2.08	143.43	134.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	CMD-C2D-C1D	2.08	130.28	126.16
28	a	419	PL9	C11-C12-C13	-2.08	105.73	111.64
23	b	609	CLA	C2D-C3D-CAD	2.08	143.42	134.94
26	B	621	SQD	O47-C45-C46	2.08	116.19	108.50
23	A	406	CLA	C3D-CAD-CBD	2.08	110.53	107.60
23	C	511	CLA	CHC-C1C-C2C	-2.08	120.94	126.51
23	b	604	CLA	C4B-C3B-C2B	-2.07	104.91	107.04
23	C	501	CLA	C2D-C3D-CAD	2.08	143.41	134.94
34	C	518	DGD	C7B-C6B-C5B	-2.07	103.55	114.56
23	B	605	CLA	O2A-CGA-CBA	2.07	118.24	111.90
23	C	507	CLA	CMD-C2D-C1D	2.07	130.26	126.16
23	B	613	CLA	CBA-CAA-C2A	-2.07	108.88	113.95
23	B	608	CLA	C2B-C3B-CAB	2.07	131.57	127.33
23	C	505	CLA	O2A-CGA-O1A	-2.07	118.07	123.48
25	C	514	BCR	C38-C26-C25	-2.07	122.16	124.50
33	B	624	HTG	O5-C5-C4	-2.07	105.88	109.73
23	c	913	CLA	CMD-C2D-C1D	2.07	130.25	126.16
23	A	410	CLA	CED-O2D-CGD	2.07	120.93	116.00
23	a	411	CLA	CED-O2D-CGD	2.07	120.93	116.00
23	B	616	CLA	C4B-C3B-CAB	-2.07	122.99	127.18
34	C	516	DGD	O2G-C1B-O1B	-2.07	118.14	123.66
25	B	618	BCR	C15-C16-C17	-2.07	118.89	123.45
28	D	405	PL9	C50-C49-C48	-2.07	115.92	122.62
23	b	612	CLA	CBC-CAC-C3C	-2.07	106.11	112.37
23	C	511	CLA	CHC-C4B-NB	2.06	128.21	124.70
23	B	606	CLA	C4-C3-C2	-2.06	119.41	123.52
24	a	413	PHO	C16-C15-C13	-2.06	109.02	115.44
23	a	414	CLA	C4D-ND-C1D	-2.06	104.08	106.57
30	b	624	LMT	O5'-C5'-C6'	2.06	111.47	106.34
23	c	907	CLA	O2D-CGD-O1D	-2.06	119.65	123.79
23	b	614	CLA	C3B-C2B-C1B	-2.06	104.41	106.69
23	c	903	CLA	C6-C5-C3	-2.06	107.92	112.62
23	b	605	CLA	C16-C17-C18	-2.06	105.17	115.69
23	b	614	CLA	C7-C6-C5	-2.06	106.96	112.97
33	b	626	HTG	O4-C4-C5	2.06	114.71	109.25
23	B	613	CLA	C2A-C3A-C4A	-2.06	98.56	101.89
30	C	520	LMT	O1B-C4'-C5'	2.06	114.68	109.35
23	d	403	CLA	CGD-CBD-CAD	-2.06	103.88	110.79
27	d	410	LMG	O7-C10-O9	-2.06	118.17	123.66
23	c	906	CLA	C11-C10-C8	-2.06	109.04	115.44
23	c	904	CLA	C4C-C3C-C2C	-2.06	103.56	106.93
23	A	407	CLA	O2A-C1-C2	-2.06	103.41	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	501	CLA	CHC-C1C-C2C	-2.06	120.98	126.51
30	B	623	LMT	O1B-C1B-O5B	2.05	115.80	110.70
23	c	908	CLA	CHB-C1B-NB	-2.06	121.22	124.70
23	c	906	CLA	CBA-CAA-C2A	2.06	118.97	113.95
23	A	405	CLA	C7-C6-C5	-2.05	106.97	112.97
23	b	614	CLA	C2A-C1A-CHA	-2.05	120.13	123.87
28	D	405	PL9	C2-C3-C4	2.05	121.73	118.81
26	B	621	SQD	O9-S-O7	-2.05	106.31	113.45
23	b	615	CLA	C5-C3-C2	-2.05	117.11	121.06
23	D	402	CLA	C16-C15-C13	2.05	121.83	115.44
23	A	405	CLA	C2A-C1A-CHA	-2.05	120.14	123.87
23	b	609	CLA	CHB-C4A-NA	2.05	127.24	124.38
25	d	404	BCR	C35-C13-C12	2.05	121.41	118.09
23	B	612	CLA	C2D-C3D-CAD	2.05	143.30	134.94
23	a	409	CLA	CMD-C2D-C1D	2.05	130.21	126.16
25	D	404	BCR	C34-C9-C8	2.05	121.40	118.09
23	b	618	CLA	C3A-C4A-CHB	-2.05	120.07	124.33
23	b	606	CLA	C1-C2-C3	-2.05	122.67	126.23
30	c	922	LMT	O2'-C2'-C1'	2.05	114.49	110.03
23	c	903	CLA	CMB-C2B-C3B	2.05	129.02	125.16
24	a	413	PHO	C2C-C1C-NC	2.05	115.27	110.51
25	B	618	BCR	C23-C22-C21	-2.04	115.83	118.98
23	B	605	CLA	C2D-C3D-CAD	2.05	143.28	134.94
23	B	613	CLA	C1-O2A-CGA	2.05	122.95	117.00
25	k	102	BCR	C20-C21-C22	-2.04	124.33	127.29
23	b	613	CLA	C2B-C1B-CHB	-2.04	122.13	126.00
23	A	407	CLA	CBC-CAC-C3C	-2.04	106.18	112.37
25	D	404	BCR	C31-C1-C2	2.04	116.90	108.78
38	H	101	RRX	C21-C20-C19	-2.04	116.37	123.23
23	C	505	CLA	C1C-NC-C4C	-2.04	103.51	106.26
23	b	616	CLA	C1C-NC-C4C	-2.04	103.51	106.26
31	B	637	GOL	O3-C3-C2	-2.04	101.29	110.37
23	B	603	CLA	C1D-CHD-C4C	-2.04	119.44	122.60
23	C	509	CLA	C4B-C3B-CAB	-2.04	123.04	127.18
23	c	913	CLA	CED-O2D-CGD	2.04	120.86	116.00
24	a	413	PHO	CMB-C2B-C1B	2.04	129.32	125.68
23	d	403	CLA	C3A-C4A-CHB	-2.04	120.09	124.33
23	a	414	CLA	CBA-CAA-C2A	-2.04	108.96	113.95
23	c	914	CLA	O2A-C1-C2	2.04	112.79	108.12
23	B	611	CLA	C6-C5-C3	-2.04	107.97	112.62
23	D	402	CLA	CHC-C4B-NB	2.04	128.16	124.70
24	a	413	PHO	C4A-NA-C1A	2.04	111.10	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C2B-C3B-CAB	2.04	131.49	127.33
34	C	516	DGD	O6D-C1D-O3G	-2.04	105.08	109.93
23	B	607	CLA	C4C-C3C-C2C	-2.04	103.59	106.93
23	b	615	CLA	C3B-CAB-CBB	-2.04	121.73	125.95
23	B	607	CLA	CBC-CAC-C3C	-2.04	106.20	112.37
24	a	413	PHO	CHC-C1C-C2C	-2.03	119.94	124.93
23	C	507	CLA	O2A-CGA-CBA	2.03	118.13	111.90
25	a	415	BCR	C15-C16-C17	-2.03	118.97	123.45
23	B	603	CLA	CMA-C3A-C4A	-2.03	105.90	112.40
24	a	413	PHO	CMB-C2B-C3B	2.03	128.99	125.16
23	C	503	CLA	C3A-C4A-NA	2.03	113.27	110.81
23	c	904	CLA	C2A-C1A-CHA	-2.03	120.17	123.87
23	B	608	CLA	CMC-C2C-C3C	2.03	131.84	126.04
23	C	509	CLA	CGD-CBD-CHA	-2.03	108.94	113.65
23	a	414	CLA	O2A-CGA-O1A	-2.03	118.17	123.48
30	m	102	LMT	C1'-O5'-C5'	2.03	117.66	113.73
23	b	616	CLA	C6-C7-C8	-2.03	109.12	115.44
23	b	618	CLA	C4B-CHC-C1C	-2.03	124.80	127.47
34	c	917	DGD	C1G-O1G-C1A	2.03	122.79	116.99
26	L	103	SQD	O47-C7-O49	-2.03	118.25	123.66
23	b	606	CLA	C3A-C4A-CHB	-2.03	120.11	124.33
33	B	631	HTG	C1-O5-C5	2.03	116.79	112.78
36	D	410	LHG	O3-C3-C2	2.03	115.09	108.54
23	C	506	CLA	C4C-C3C-C2C	-2.03	103.61	106.93
27	c	921	LMG	C9-C8-C7	-2.03	107.20	111.86
23	c	911	CLA	C4B-CHC-C1C	-2.03	124.80	127.47
23	b	608	CLA	C1D-CHD-C4C	2.03	125.74	122.60
33	d	401	HTG	O5-C1-C2	2.03	113.03	110.42
30	a	402	LMT	O5'-C1'-C2'	-2.03	106.16	110.30
30	m	101	LMT	O2B-C2B-C1B	-2.03	105.63	110.03
34	d	406	DGD	O2D-C2D-C3D	2.03	114.88	110.36
23	A	405	CLA	OBD-CAD-C3D	-2.02	124.06	128.15
34	C	517	DGD	O3D-C3D-C2D	-2.02	105.83	110.36
23	b	609	CLA	C2B-C1B-CHB	-2.03	122.16	126.00
31	b	632	GOL	O1-C1-C2	2.02	119.36	110.37
23	C	504	CLA	C2A-C1A-CHA	-2.02	120.19	123.87
30	J	102	LMT	O5'-C5'-C6'	2.02	111.38	106.34
23	d	402	CLA	O2D-CGD-CBD	2.02	115.43	111.34
23	c	911	CLA	C1D-CHD-C4C	-2.02	119.46	122.60
23	C	502	CLA	CMA-C3A-C4A	-2.02	105.94	112.40
25	k	101	BCR	C16-C15-C14	-2.02	118.99	123.45
23	b	617	CLA	C4D-C3D-CAD	2.02	110.54	108.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	m	101	LMT	C1B-O5B-C5B	2.02	117.64	113.73
23	a	414	CLA	C1D-CHD-C4C	-2.02	119.47	122.60
26	B	621	SQD	C45-O47-C7	2.02	122.60	117.86
23	b	607	CLA	O2A-CGA-CBA	2.02	118.08	111.90
33	B	626	HTG	O5-C5-C4	-2.02	105.98	109.73
23	b	609	CLA	C1-C2-C3	-2.02	122.72	126.23
23	d	403	CLA	CHB-C4A-NA	2.02	127.19	124.38
23	A	410	CLA	O2A-CGA-CBA	2.02	118.08	111.90
23	c	902	CLA	CHB-C4A-NA	2.02	127.19	124.38
25	B	620	BCR	C16-C15-C14	-2.02	119.00	123.45
38	H	101	RRX	C29-C28-C27	-2.02	106.50	110.29
38	H	101	RRX	C38-C26-C25	-2.02	122.22	124.50
23	d	403	CLA	CMC-C2C-C3C	2.02	131.79	126.04
24	a	413	PHO	C4B-NB-C1B	-2.02	104.65	108.29
24	A	409	PHO	O2D-CGD-CBD	2.02	115.41	111.34
24	A	408	PHO	C3B-C4B-NB	2.02	114.89	107.09
23	B	614	CLA	CAA-CBA-CGA	-2.02	107.30	113.24
23	c	906	CLA	O2A-CGA-CBA	2.01	118.06	111.90
23	c	906	CLA	OBD-CAD-C3D	-2.01	124.08	128.15
23	B	614	CLA	O2A-CGA-CBA	2.02	118.07	111.90
23	A	405	CLA	OBD-CAD-CBD	2.01	128.98	125.94
23	B	602	CLA	C4D-ND-C1D	-2.01	104.14	106.57
23	C	509	CLA	C4C-C3C-C2C	-2.01	103.63	106.93
34	C	518	DGD	C3A-C2A-C1A	-2.01	105.71	113.51
23	C	501	CLA	CHB-C4A-NA	2.01	127.19	124.38
23	c	913	CLA	C4C-C3C-C2C	-2.01	103.64	106.93
23	b	617	CLA	C5-C3-C2	2.01	124.92	121.06
23	a	410	CLA	C4D-ND-C1D	-2.01	104.14	106.57
27	D	411	LMG	O4-C4-C3	-2.01	105.87	110.36
23	c	914	CLA	C2A-C1A-CHA	-2.01	120.22	123.87
30	m	101	LMT	C10-C9-C8	-2.01	103.90	114.56
23	c	910	CLA	C4D-CHA-C1A	-2.01	114.50	120.32
30	M	102	LMT	O5'-C5'-C6'	2.01	111.33	106.34
25	c	915	BCR	C8-C7-C6	-2.01	121.31	127.23
23	a	414	CLA	O2A-C1-C2	2.01	112.71	108.12
26	L	103	SQD	C28-C27-C26	-2.01	103.91	114.56
23	B	604	CLA	C4B-C3B-CAB	-2.01	123.12	127.18
23	C	502	CLA	C4C-C3C-C2C	-2.00	103.64	106.93
23	C	505	CLA	C3A-C4A-NA	2.00	113.23	110.81
23	A	407	CLA	C2D-C3D-CAD	2.01	143.12	134.94
28	A	414	PL9	C26-C24-C23	2.01	124.92	121.06
23	B	608	CLA	CAC-C3C-C4C	2.01	127.86	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	921	LMG	O6-C5-C6	2.00	111.33	106.34
23	B	608	CLA	CAA-CBA-CGA	-2.00	107.33	113.24
23	A	406	CLA	C4-C3-C2	-2.00	119.53	123.52
23	B	615	CLA	C1C-C2C-C3C	-2.00	104.44	106.96
23	B	617	CLA	CHB-C1B-NB	-2.00	121.31	124.70
36	E	101	LHG	O8-C23-C24	2.00	118.03	111.90
24	A	408	PHO	CMD-C2D-C3D	2.00	128.93	125.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.17	4 (1%) 75 78	16, 23, 46, 69	0
1	a	334/344 (97%)	0.00	13 (3%) 37 38	19, 24, 50, 76	0
2	B	504/504 (100%)	0.06	29 (5%) 22 22	18, 27, 54, 88	0
2	b	501/504 (99%)	0.10	38 (7%) 14 13	20, 29, 58, 119	0
3	C	451/455 (99%)	-0.10	8 (1%) 65 67	21, 31, 46, 81	0
3	c	455/455 (100%)	0.11	20 (4%) 33 33	23, 34, 48, 79	0
4	D	340/342 (99%)	-0.21	3 (0%) 81 83	17, 24, 40, 70	0
4	d	340/342 (99%)	-0.20	5 (1%) 70 72	19, 26, 45, 80	0
5	E	81/83 (97%)	0.82	17 (20%) 1 1	27, 40, 62, 82	0
5	e	79/83 (95%)	0.92	11 (13%) 4 3	32, 44, 72, 82	0
6	F	34/44 (77%)	0.21	5 (14%) 3 3	26, 34, 63, 74	0
6	f	32/44 (72%)	0.13	2 (6%) 19 19	29, 37, 76, 86	0
7	H	63/63 (100%)	-0.03	1 (1%) 68 70	24, 33, 43, 70	0
7	h	63/63 (100%)	0.35	2 (3%) 45 46	27, 37, 51, 81	0
8	I	36/38 (94%)	-0.28	0 100 100	27, 34, 64, 86	0
8	i	38/38 (100%)	0.12	2 (5%) 25 26	26, 34, 71, 83	0
9	J	36/40 (90%)	0.07	3 (8%) 11 11	26, 38, 65, 79	0
9	j	39/40 (97%)	0.31	5 (12%) 4 4	30, 42, 68, 84	0
10	K	37/37 (100%)	-0.23	0 100 100	32, 38, 47, 63	0
10	k	37/37 (100%)	0.03	1 (2%) 52 53	36, 42, 55, 69	0
11	L	37/37 (100%)	-0.11	3 (8%) 12 11	17, 22, 65, 75	0
11	l	37/37 (100%)	0.11	3 (8%) 12 11	19, 23, 64, 95	0
12	M	33/36 (91%)	-0.28	1 (3%) 48 49	21, 24, 40, 56	0
12	m	34/36 (94%)	-0.13	1 (2%) 49 50	20, 25, 48, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	0.43	31 (12%) 4 4	18, 33, 66, 120	0
13	o	241/244 (98%)	0.36	35 (14%) 3 3	20, 35, 71, 87	0
14	T	30/32 (93%)	-0.13	1 (3%) 44 45	19, 23, 49, 85	0
14	t	30/32 (93%)	-0.03	1 (3%) 44 45	20, 24, 47, 72	0
15	U	97/104 (93%)	-0.06	1 (1%) 79 81	23, 30, 52, 58	0
15	u	97/104 (93%)	-0.36	1 (1%) 79 81	24, 30, 40, 66	0
16	V	137/137 (100%)	-0.28	0 100 100	22, 28, 43, 51	0
16	v	137/137 (100%)	0.41	11 (8%) 12 12	26, 37, 52, 72	0
17	Y	27/30 (90%)	0.94	5 (18%) 2 2	37, 47, 70, 77	0
17	y	28/30 (93%)	1.10	6 (21%) 1 1	45, 55, 73, 77	0
18	X	38/40 (95%)	0.58	7 (18%) 2 2	32, 39, 65, 69	0
18	x	38/40 (95%)	1.02	8 (21%) 1 1	34, 42, 83, 94	0
19	Z	62/62 (100%)	1.51	20 (32%) 1 1	37, 46, 75, 92	0
19	z	60/62 (96%)	1.80	23 (38%) 1 1	47, 57, 88, 95	0
All	All	5241/5344 (98%)	0.10	327 (6%) 20 20	16, 30, 59, 120	0

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	37	VAL	7.7
2	b	496	TYR	7.5
18	x	38	GLN	7.3
13	o	246	ALA	7.0
2	b	489	GLU	6.6
2	B	494	GLY	6.4
2	b	487	SER	6.4
2	B	495	PHE	6.2
13	O	60	ARG	6.2
19	Z	3	ILE	6.0
2	b	488	PRO	6.0
19	Z	62	VAL	5.8
19	Z	7	LEU	5.7
17	y	19	ILE	5.7
13	O	25	THR	5.6
19	z	61	VAL	5.6
19	z	2	THR	5.6
2	b	484	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
19	Z	32	ASP	5.5
11	l	1	MET	5.4
18	x	2	THR	5.4
19	z	4	LEU	5.4
17	Y	22	LEU	5.3
19	Z	31	GLN	5.3
1	A	11	ALA	5.2
19	Z	33	TRP	5.2
2	b	495	PHE	5.2
13	o	25	THR	5.2
2	b	494	GLY	5.1
2	b	502	VAL	5.1
19	z	5	PHE	5.1
19	z	60	PHE	5.1
2	B	486	LEU	5.0
2	B	487	SER	4.8
2	b	500	GLY	4.8
9	J	5	GLY	4.8
19	Z	4	LEU	4.8
5	E	21	VAL	4.8
2	b	503	THR	4.7
2	B	496	TYR	4.7
19	Z	30	PRO	4.7
5	E	17	VAL	4.7
2	b	85	GLY	4.6
18	X	2	THR	4.6
2	b	499	VAL	4.5
13	O	3	GLN	4.5
2	b	86	ILE	4.5
13	O	27	ARG	4.5
5	e	25	ILE	4.4
2	b	126	PRO	4.4
13	o	36	GLN	4.3
19	z	33	TRP	4.3
13	o	23	ASP	4.3
5	E	84	LYS	4.3
13	o	35	SER	4.3
1	a	13	LEU	4.3
19	z	7	LEU	4.3
6	f	14	PRO	4.3
13	o	243	ILE	4.3
17	y	20	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	b	490	GLN	4.2
5	E	83	LEU	4.2
3	C	23	ALA	4.2
5	E	6	GLY	4.1
9	j	6	GLY	4.1
5	E	4	THR	4.1
19	Z	34	ASP	4.1
13	O	133	VAL	4.0
9	J	6	GLY	4.0
2	B	500	GLY	4.0
13	O	26	ALA	4.0
13	o	26	ALA	4.0
13	O	4	THR	4.0
16	v	26	TYR	3.9
3	C	143	TYR	3.9
2	b	493	TRP	3.8
13	O	24	ASP	3.8
17	y	22	LEU	3.8
6	F	12	SER	3.8
9	j	5	GLY	3.8
11	L	1	MET	3.8
6	F	16	PHE	3.7
13	O	23	ASP	3.7
4	d	238	THR	3.7
19	z	6	GLN	3.7
7	h	64	ALA	3.7
19	z	3	ILE	3.7
2	B	490	GLN	3.7
13	O	58	ASN	3.7
19	Z	1	MET	3.6
15	u	8	GLU	3.6
3	C	24	THR	3.6
13	o	38	TYR	3.6
4	d	12	ARG	3.6
10	k	18	PHE	3.6
13	o	58	ASN	3.5
11	L	3	PRO	3.5
19	Z	60	PHE	3.5
2	b	161	LEU	3.5
2	B	501	ASP	3.5
9	j	8	ILE	3.5
13	o	32	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
3	c	201[A]	ASN	3.4
2	B	293	ALA	3.4
2	b	293	ALA	3.4
2	b	497	GLN	3.4
4	D	238	THR	3.3
2	b	504	THR	3.3
14	t	29	ILE	3.3
1	A	13	LEU	3.3
5	e	83	LEU	3.3
3	c	279	LEU	3.3
2	B	485	GLU	3.3
6	F	13	TYR	3.3
2	b	492	GLU	3.3
5	e	84	LYS	3.2
1	a	11	ALA	3.2
18	x	39	ARG	3.2
16	v	14	SER	3.2
2	b	295	GLY	3.2
2	B	503	THR	3.2
16	v	19	ILE	3.2
18	x	3	ILE	3.2
14	T	30	THR	3.2
16	v	8	LEU	3.2
16	v	21	LEU	3.2
6	F	15	ILE	3.2
13	O	132	ASN	3.2
1	a	235	TYR	3.1
2	B	484	PRO	3.1
19	Z	35	ARG	3.1
19	z	39	LEU	3.1
2	B	504	THR	3.1
2	b	298	LEU	3.1
5	e	61	ARG	3.1
2	B	488	PRO	3.1
11	l	3	PRO	3.1
4	d	240	ALA	3.1
2	B	502	VAL	3.0
2	B	295	GLY	3.0
3	c	200	THR	3.0
2	b	491	VAL	3.0
19	z	53	VAL	3.0
4	d	237	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
5	E	20	TRP	3.0
9	j	4	GLU	3.0
5	e	6	GLY	3.0
7	H	64	ALA	3.0
13	O	32	ILE	3.0
13	O	57	LYS	3.0
13	O	56	PRO	2.9
13	o	141[A]	ASP	2.9
13	o	34	SER	2.9
1	a	242	GLU	2.9
18	X	38	GLN	2.9
18	X	3	ILE	2.9
19	z	46	LEU	2.9
13	o	89	SER	2.9
13	o	4	THR	2.9
13	o	30	TYR	2.9
2	b	84	THR	2.9
2	B	499	VAL	2.9
3	c	21	ILE	2.8
3	c	19	ASN	2.8
13	o	24	ASP	2.8
13	o	27	ARG	2.8
18	X	37	VAL	2.8
19	Z	61	VAL	2.8
4	D	13	GLY	2.8
2	b	297	THR	2.8
2	B	483	ASP	2.8
18	x	36	LYS	2.8
3	c	433	LEU	2.8
18	X	34	ILE	2.8
19	z	32	ASP	2.7
2	B	2	GLY	2.7
3	c	20	SER	2.7
12	M	33	GLN	2.7
9	J	8	ILE	2.7
16	v	10	VAL	2.7
2	B	497	GLN	2.7
12	m	34	LYS	2.7
13	O	89	SER	2.7
13	o	33	ASP	2.7
2	b	292	LEU	2.7
13	O	88	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
13	o	87	VAL	2.7
18	x	34	ILE	2.7
2	b	296	ALA	2.6
17	y	21	GLN	2.6
19	z	57	LEU	2.6
2	B	297	THR	2.6
5	E	5	THR	2.6
13	O	87	VAL	2.6
17	Y	41	VAL	2.6
13	o	22	LEU	2.6
13	o	132	ASN	2.6
18	X	31	ILE	2.6
3	c	434	ALA	2.6
13	o	245	PRO	2.6
13	O	130	GLN	2.6
19	Z	36	SER	2.6
2	B	489	GLU	2.6
6	F	14	PRO	2.6
13	o	134	THR	2.6
5	E	19	TYR	2.6
2	b	294	SER	2.6
19	z	41	PHE	2.6
13	O	207	ARG	2.6
1	A	12	ASN	2.6
3	C	25	ASN	2.6
2	b	128	THR	2.5
2	b	129	GLY	2.5
16	v	15	GLU	2.5
13	O	136	ILE	2.5
13	o	207	ARG	2.5
2	B	161	LEU	2.5
1	a	12	ASN	2.5
13	o	209	GLY	2.5
13	o	57	LYS	2.5
17	y	37	PHE	2.5
3	C	262	ARG	2.5
8	i	34	ARG	2.5
11	l	2	GLU	2.5
5	e	26	THR	2.4
13	o	37	THR	2.4
3	c	429	SER	2.4
7	h	6	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	15	THR	2.4
2	B	296	ALA	2.4
5	E	81	GLU	2.4
3	c	143	TYR	2.4
5	e	28	PRO	2.4
13	O	91	GLY	2.4
16	v	16	GLY	2.4
16	v	12	LEU	2.4
2	B	294	SER	2.4
17	Y	40	ALA	2.4
8	i	37	LEU	2.4
19	Z	2	THR	2.4
13	O	135	SER	2.4
19	z	9	LEU	2.4
5	E	82	GLN	2.4
2	b	301	ALA	2.4
1	a	240	GLY	2.4
16	v	22	THR	2.4
4	D	12	ARG	2.3
19	z	31	GLN	2.3
13	O	131	PRO	2.3
19	Z	5	PHE	2.3
2	b	127	ARG	2.3
3	c	426	LEU	2.3
3	c	437	PHE	2.3
3	c	425	TRP	2.3
15	U	8	GLU	2.3
13	O	28	GLY	2.3
3	c	432	VAL	2.3
1	a	264	SER	2.3
3	c	280	SER	2.3
5	e	32	ILE	2.3
19	z	8	ALA	2.3
13	O	62	GLU	2.3
17	Y	21	GLN	2.3
19	Z	29	SER	2.3
5	e	59	GLU	2.2
19	z	30	PRO	2.2
19	z	10	ALA	2.2
13	o	85	LEU	2.2
17	y	25	ILE	2.2
18	X	39	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	501	ASP	2.2
13	O	61	GLN	2.2
19	Z	40	ILE	2.2
19	z	43	GLY	2.2
2	b	483	ASP	2.2
5	E	80	LEU	2.2
13	O	22	LEU	2.2
3	c	191	PRO	2.2
1	a	14	TRP	2.2
18	x	35	ASP	2.2
5	e	21	VAL	2.2
6	f	16	PHE	2.2
13	o	244	GLU	2.2
3	C	207	ARG	2.2
3	c	253	LEU	2.2
13	O	93	LEU	2.2
5	e	29	ALA	2.2
19	z	59	PHE	2.2
19	Z	42	LEU	2.2
19	z	34	ASP	2.1
13	o	133	VAL	2.1
5	E	22	ILE	2.1
5	E	25	ILE	2.1
13	o	204	VAL	2.1
1	a	225	ARG	2.1
2	b	458	PHE	2.1
3	C	257	PHE	2.1
5	E	61	ARG	2.1
1	a	266	ASN	2.1
1	a	16	ARG	2.1
13	o	5	LEU	2.1
13	O	137	THR	2.1
3	c	155	ASN	2.1
2	B	457	VAL	2.1
13	o	208	THR	2.1
19	Z	6	GLN	2.1
9	j	12	ILE	2.1
13	o	39	ARG	2.1
1	A	243	GLU	2.1
2	B	402	TYR	2.1
13	o	28	GLY	2.1
1	a	280	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	b	122	LEU	2.0
3	C	204	LEU	2.0
2	B	405[A]	GLU	2.0
3	c	142	GLU	2.0
5	E	18	ARG	2.0
16	v	18	THR	2.0
13	O	92	SER	2.0
17	Y	42	ARG	2.0
4	d	154	VAL	2.0
1	a	243	GLU	2.0
3	c	427	ALA	2.0
13	O	138	THR	2.0
2	b	125	ASP	2.0
2	B	352[A]	GLU	2.0
11	L	2	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	HSK	D	336[B]	8/12	0.11	3.42	23,26,27,29	8
4	HSK	D	336[A]	7/12	0.11	3.42	26,30,31,34	7
12	FME	m	1	10/11	0.12	1.59	31,38,54,60	0
4	HSK	d	336[B]	8/12	0.10	1.56	30,34,37,38	8
4	HSK	d	336[A]	7/12	0.10	1.44	30,39,40,44	7
14	FME	t	1	10/11	0.10	1.22	20,23,41,50	0
14	FME	T	1	10/11	0.09	0.82	24,27,43,50	0
12	FME	M	1	10/11	0.10	0.66	27,34,51,59	0
8	FME	i	1	10/11	0.12	0.33	30,32,37,39	0
8	FME	I	1	10/11	0.08	-0.30	27,34,38,39	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
29	UNL	T	102	13/-	0.47	36.36	66,70,83,87	0
29	UNL	A	420	4/-	0.42	30.25	64,66,66,66	0
31	GOL	b	633	6/6	0.33	19.94	41,46,49,52	0
29	UNL	a	403	6/-	0.38	13.90	57,62,66,66	0
31	GOL	D	415	6/6	0.18	11.33	35,36,42,46	0
29	UNL	M	103	16/-	0.21	11.24	49,58,77,79	0
29	UNL	t	103	16/-	0.40	11.00	63,74,94,95	0
31	GOL	c	928	6/6	0.26	10.05	42,51,54,54	0
40	SO4	O	302	5/5	0.29	10.00	78,87,95,105	0
29	UNL	b	628	36/-	0.25	9.63	44,65,101,106	0
33	HTG	B	626	19/19	0.39	9.43	48,87,92,93	0
29	UNL	b	631	16/-	0.29	9.28	59,66,77,79	0
33	HTG	b	602	19/19	0.31	9.08	50,93,111,117	0
30	LMT	b	625	24/35	0.23	8.32	35,61,99,100	0
31	GOL	C	526	6/6	0.15	7.88	38,43,51,57	0
29	UNL	E	102	15/-	0.27	7.62	57,64,83,83	0
29	UNL	C	523	34/-	0.23	7.23	52,77,88,93	0
29	UNL	d	411	16/-	0.28	7.22	39,49,63,66	0
29	UNL	c	926	10/-	0.21	6.92	65,67,71,72	0
33	HTG	d	401	19/19	0.29	6.79	55,101,111,114	0
31	GOL	L	104	6/6	0.24	6.53	44,52,54,55	0
34	DGD	d	406	50/66	0.30	6.24	56,75,94,97	0
31	GOL	l	102	6/6	0.34	6.23	37,55,57,57	0
34	DGD	D	406	53/66	0.30	6.06	53,77,92,103	0
29	UNL	D	413	16/-	0.24	5.96	39,47,65,65	0
29	UNL	A	416	16/-	0.15	5.76	41,46,73,73	0
30	LMT	F	102	35/35	0.41	5.65	53,84,91,96	0
29	UNL	B	629	14/-	0.29	5.58	61,70,89,90	0
29	UNL	B	628	10/-	0.35	5.25	52,56,70,74	0
31	GOL	V	205	6/6	0.31	5.15	33,36,37,41	0
30	LMT	J	102	24/35	0.18	5.13	45,55,79,83	0
29	UNL	i	103	13/-	0.33	4.97	58,65,76,78	0
29	UNL	B	632	16/-	0.40	4.86	50,59,73,73	0
29	UNL	b	630	16/-	0.43	4.77	51,62,73,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	GOL	f	104	6/6	0.36	4.66	46,51,51,54	0
23	CLA	b	604	65/65	0.19	4.52	34,47,73,81	0
29	UNL	i	104	10/-	0.33	4.39	67,72,77,78	0
27	LMG	c	921	51/55	0.34	4.38	38,80,95,111	0
33	HTG	C	522	19/19	0.31	4.31	50,79,92,94	0
29	UNL	i	101	16/-	0.12	4.30	40,46,56,62	0
29	UNL	j	102	16/-	0.16	4.25	52,61,69,69	0
30	LMT	t	102	24/35	0.22	4.20	33,55,94,95	0
29	UNL	E	103	12/-	0.26	4.17	65,73,83,88	0
33	HTG	D	414	19/19	0.38	4.10	66,93,106,107	0
31	GOL	C	524	6/6	0.17	4.01	36,45,47,53	0
33	HTG	B	631	19/19	0.20	4.00	49,111,120,125	0
31	GOL	V	204	6/6	0.27	3.97	39,52,59,59	0
23	CLA	B	602	65/65	0.21	3.61	29,41,78,95	0
33	HTG	c	924	19/19	0.47	3.56	53,85,97,100	0
29	UNL	z	102	16/-	0.30	3.53	51,70,89,92	0
30	LMT	M	101	35/35	0.23	3.46	43,61,77,90	0
31	GOL	b	632	6/6	0.11	3.45	35,42,46,47	0
33	HTG	b	626	19/19	0.17	3.38	29,40,73,75	0
28	PL9	A	414	55/55	0.24	3.37	47,66,93,96	0
27	LMG	A	413	51/55	0.21	3.34	42,57,76,78	0
26	SQD	a	401	54/54	0.17	3.34	45,59,85,90	0
29	UNL	X	101	16/-	0.13	3.29	34,39,58,60	0
29	UNL	I	102	11/-	0.26	3.26	62,65,66,68	0
33	HTG	V	202	13/19	0.27	3.16	43,48,76,84	0
29	UNL	c	925	30/-	0.16	3.13	59,72,89,95	0
29	UNL	e	800	11/-	0.33	3.12	53,60,68,68	0
36	LHG	d	407	49/49	0.20	3.12	27,36,46,49	0
29	UNL	D	412	40/-	0.19	3.10	39,60,96,99	0
31	GOL	c	930	6/6	0.28	3.09	49,54,57,59	0
28	PL9	a	419	55/55	0.26	3.06	52,74,98,109	0
26	SQD	L	103	54/54	0.21	3.04	43,64,89,96	0
29	UNL	A	417	13/-	0.35	3.03	56,59,66,66	0
26	SQD	A	418	54/54	0.15	3.02	42,59,81,86	0
33	HTG	u	201	14/19	0.25	2.95	46,64,90,96	0
31	GOL	a	424	6/6	0.20	2.94	42,56,59,74	0
31	GOL	a	422	6/6	0.12	2.94	30,38,44,45	0
29	UNL	i	102	16/-	0.24	2.83	54,65,83,84	0
31	GOL	A	423	6/6	0.23	2.82	39,43,45,53	0
26	SQD	B	621	54/54	0.22	2.80	48,65,108,109	0
31	GOL	B	633	6/6	0.11	2.76	34,39,47,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	DGD	C	518	62/66	0.13	2.64	20,30,68,75	0
31	GOL	B	638	6/6	0.13	2.64	35,47,49,53	0
29	UNL	a	420	40/-	0.38	2.61	53,72,88,94	0
30	LMT	c	922	35/35	0.32	2.60	61,73,85,90	0
33	HTG	b	601	19/19	0.15	2.56	43,51,62,68	0
33	HTG	c	923	19/19	0.23	2.55	64,75,82,83	0
29	UNL	H	103	10/-	0.24	2.55	60,69,74,76	0
29	UNL	a	421	10/-	0.32	2.51	53,57,61,64	0
36	LHG	a	417	40/49	0.24	2.50	60,109,148,151	0
31	GOL	A	422	6/6	0.14	2.50	42,55,58,67	0
36	LHG	D	410	46/49	0.13	2.48	24,32,82,87	0
31	GOL	a	423	6/6	0.10	2.46	33,34,35,45	0
26	SQD	D	407	45/54	0.31	2.44	50,78,94,101	0
30	LMT	A	419	35/35	0.14	2.30	37,56,73,94	0
27	LMG	Z	101	51/55	0.29	2.20	41,76,102,113	0
29	UNL	I	101	13/-	0.24	2.20	44,53,61,63	0
39	MG	j	101	1/1	0.15	2.18	35,35,35,35	0
31	GOL	B	636	6/6	0.16	2.14	33,43,47,56	0
33	HTG	U	201	9/19	0.26	2.12	54,59,82,98	0
31	GOL	c	927	6/6	0.13	2.12	43,53,60,68	0
29	UNL	x	101	16/-	0.15	2.07	36,45,70,73	0
27	LMG	D	411	51/55	0.16	2.06	23,35,91,99	0
29	UNL	J	104	12/-	0.17	2.02	53,65,72,74	0
30	LMT	z	101	32/35	0.26	1.99	46,85,90,100	0
29	UNL	A	415	36/-	0.29	1.86	58,67,75,79	0
29	UNL	j	103	12/-	0.28	1.86	55,65,70,71	0
30	LMT	C	520	35/35	0.26	1.83	52,71,83,89	0
27	LMG	d	410	51/55	0.11	1.79	29,36,80,91	0
31	GOL	O	304	6/6	0.21	1.78	52,60,61,63	0
30	LMT	Z	102	35/35	0.27	1.74	41,87,102,107	0
25	BCR	D	404	40/40	0.17	1.73	24,29,55,57	0
23	CLA	c	909	65/65	0.19	1.65	25,30,82,98	0
31	GOL	b	635	6/6	0.14	1.65	40,43,46,48	0
34	DGD	C	516	62/66	0.17	1.63	22,32,85,87	0
30	LMT	m	102	35/35	0.16	1.60	41,54,72,84	0
25	BCR	B	618	40/40	0.14	1.57	20,26,29,30	0
36	LHG	D	408	49/49	0.13	1.55	26,35,45,45	0
23	CLA	C	510	65/65	0.16	1.55	22,28,38,41	0
30	LMT	b	624	25/35	0.18	1.55	51,71,94,98	0
33	HTG	B	625	19/19	0.20	1.55	31,38,71,75	0
23	CLA	C	508	65/65	0.14	1.53	24,29,73,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	BCR	B	619	40/40	0.17	1.53	19,26,42,45	0
28	PL9	d	405	55/55	0.15	1.50	19,25,30,34	0
25	BCR	d	404	40/40	0.10	1.48	25,33,56,58	0
27	LMG	a	418	51/55	0.18	1.47	43,60,68,73	0
23	CLA	B	611	65/65	0.13	1.46	19,25,34,39	0
29	UNL	Z	103	16/-	0.24	1.40	48,63,81,81	0
25	BCR	T	101	40/40	0.13	1.39	24,32,47,53	0
34	DGD	H	102	62/66	0.18	1.38	24,31,40,45	0
27	LMG	B	622	51/55	0.16	1.38	28,37,53,63	0
23	CLA	b	614	65/65	0.17	1.36	20,24,36,45	0
23	CLA	C	509	65/65	0.13	1.36	27,31,47,51	0
23	CLA	c	914	65/65	0.17	1.36	38,53,90,98	0
36	LHG	d	409	49/49	0.15	1.34	27,32,85,91	0
24	PHO	a	413	64/64	0.13	1.34	19,25,30,35	0
23	CLA	C	505	65/65	0.13	1.32	26,31,47,51	0
23	CLA	b	611	65/65	0.17	1.30	22,27,39,43	0
30	LMT	a	402	35/35	0.15	1.29	37,54,69,80	0
23	CLA	A	410	65/65	0.11	1.28	20,24,99,105	0
36	LHG	E	101	49/49	0.21	1.25	50,80,94,97	0
33	HTG	b	627	19/19	0.36	1.22	53,94,104,105	0
30	LMT	M	102	35/35	0.19	1.20	35,52,60,63	0
23	CLA	A	407	65/65	0.13	1.18	18,21,80,92	0
25	BCR	C	515	40/40	0.12	1.18	28,34,41,44	0
36	LHG	D	409	49/49	0.11	1.17	22,28,40,44	0
31	GOL	A	421	6/6	0.12	1.16	30,37,38,41	0
26	SQD	A	412	54/54	0.12	1.14	35,54,71,74	0
31	GOL	V	203	6/6	0.14	1.12	26,32,36,38	0
36	LHG	l	101	49/49	0.15	1.11	22,31,47,57	0
36	LHG	d	408	49/49	0.12	1.11	22,27,42,47	0
29	UNL	L	102	14/-	0.21	1.10	52,58,66,69	0
23	CLA	c	911	65/65	0.23	1.10	24,30,41,45	0
31	GOL	b	636	6/6	0.11	1.10	45,56,58,60	0
31	GOL	C	525	6/6	0.13	1.04	26,26,27,29	0
27	LMG	b	623	51/55	0.15	1.03	30,39,52,63	0
23	CLA	a	411	65/65	0.13	1.03	18,23,106,117	0
23	CLA	B	613	65/65	0.14	1.02	19,24,31,34	0
23	CLA	C	503	65/65	0.13	1.02	26,31,38,39	0
31	GOL	B	637	6/6	0.13	1.01	36,38,45,54	0
36	LHG	L	101	49/49	0.12	0.98	22,31,44,49	0
23	CLA	B	605	65/65	0.17	0.93	19,22,53,55	0
26	SQD	a	416	54/54	0.14	0.91	37,55,88,90	0
23	CLA	c	910	65/65	0.18	0.91	25,31,49,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	B	608	65/65	0.14	0.90	17,20,34,37	0
23	CLA	B	612	65/65	0.12	0.90	18,21,34,37	0
34	DGD	C	517	62/66	0.12	0.90	22,31,78,92	0
31	GOL	v	204	6/6	0.24	0.89	46,50,61,62	0
30	LMT	B	623	35/35	0.21	0.88	43,79,117,129	0
27	LMG	c	920	51/55	0.21	0.88	30,65,100,104	0
23	CLA	b	616	65/65	0.19	0.88	20,24,46,50	0
34	DGD	c	919	62/66	0.13	0.88	25,35,60,71	0
32	CA	b	603	1/1	0.07	0.88	82,82,82,82	0
25	BCR	A	411	40/40	0.11	0.87	21,26,33,36	0
23	CLA	b	613	65/65	0.13	0.86	24,28,35,40	0
31	GOL	B	635	6/6	0.12	0.86	38,47,49,50	0
32	CA	F	103	1/1	0.15	0.82	55,55,55,55	0
34	DGD	h	102	62/66	0.15	0.82	27,35,45,52	0
23	CLA	a	414	65/65	0.10	0.81	19,25,99,104	0
25	BCR	b	620	40/40	0.14	0.80	23,27,33,33	0
25	BCR	b	621	40/40	0.16	0.79	21,28,43,46	0
23	CLA	b	612	65/65	0.12	0.78	26,30,36,38	0
24	PHO	A	409	64/64	0.14	0.76	19,22,29,37	0
27	LMG	C	519	51/55	0.16	0.75	29,59,97,105	0
23	CLA	B	609	65/65	0.14	0.75	18,24,31,34	0
33	HTG	C	521	19/19	0.16	0.74	56,63,76,80	0
23	CLA	d	402	65/65	0.12	0.73	18,21,39,44	0
25	BCR	t	101	40/40	0.13	0.72	23,30,42,44	0
26	SQD	f	102	33/54	0.20	0.71	63,73,113,114	0
23	CLA	b	607	65/65	0.16	0.71	20,25,54,59	0
23	CLA	C	502	65/65	0.15	0.71	21,26,39,48	0
23	CLA	b	617	65/65	0.13	0.66	20,25,71,83	0
23	CLA	c	903	65/65	0.20	0.65	22,29,42,55	0
23	CLA	a	410	65/65	0.12	0.64	17,20,28,34	0
23	CLA	B	617	65/65	0.11	0.64	20,28,79,83	0
23	CLA	C	501	65/65	0.13	0.64	25,32,46,53	0
33	HTG	B	630	19/19	0.12	0.63	39,52,66,79	0
23	CLA	C	504	65/65	0.13	0.62	23,28,62,68	0
23	CLA	B	614	65/65	0.15	0.62	18,23,48,54	0
25	BCR	b	622	40/40	0.10	0.61	25,33,43,45	0
34	DGD	c	917	62/66	0.14	0.59	24,33,77,80	0
23	CLA	b	606	65/65	0.12	0.59	20,26,37,42	0
25	BCR	K	101	40/40	0.10	0.58	30,35,40,43	0
23	CLA	B	610	65/65	0.11	0.52	23,28,33,35	0
23	CLA	c	902	65/65	0.12	0.52	27,34,46,50	0
23	CLA	B	606	65/65	0.14	0.51	17,23,35,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	C	513	65/65	0.14	0.50	35,46,78,83	0
23	CLA	B	604	65/65	0.13	0.50	17,22,34,41	0
29	UNL	B	627	16/-	0.13	0.50	43,47,69,69	0
30	LMT	m	101	35/35	0.18	0.49	32,51,61,62	0
23	CLA	c	908	65/65	0.12	0.47	26,32,52,55	0
23	CLA	c	904	65/65	0.15	0.46	24,37,42,42	0
37	HEM	f	101	43/43	0.16	0.45	39,47,61,77	0
25	BCR	k	102	40/40	0.13	0.44	29,41,48,50	0
23	CLA	b	610	65/65	0.12	0.41	18,23,32,35	0
38	RRX	H	101	41/41	0.15	0.40	25,30,44,47	0
23	CLA	b	608	65/65	0.11	0.40	20,24,33,34	0
28	PL9	D	405	55/55	0.08	0.39	18,23,31,38	0
23	CLA	a	409	65/65	0.12	0.39	18,21,31,43	0
31	GOL	v	203	6/6	0.14	0.36	31,35,41,43	0
23	CLA	B	603	65/65	0.13	0.35	23,26,34,37	0
23	CLA	A	406	65/65	0.09	0.33	13,18,29,39	0
23	CLA	b	615	65/65	0.14	0.33	19,27,33,38	0
23	CLA	C	506	65/65	0.12	0.33	25,38,94,97	0
24	PHO	A	408	64/64	0.10	0.31	16,21,25,27	0
23	CLA	c	905	65/65	0.17	0.31	24,31,64,66	0
23	CLA	c	913	65/65	0.11	0.28	33,45,67,72	0
23	CLA	C	512	65/65	0.10	0.27	34,41,69,74	0
23	CLA	B	616	65/65	0.10	0.27	23,28,48,50	0
31	GOL	b	634	6/6	0.10	0.24	32,39,44,46	0
29	UNL	J	103	14/-	0.15	0.21	61,66,73,76	0
23	CLA	D	402	65/65	0.10	0.18	13,18,36,39	0
31	GOL	c	929	6/6	0.13	0.17	25,27,30,30	0
25	BCR	c	915	40/40	0.12	0.13	44,51,59,60	0
23	CLA	A	405	65/65	0.09	0.11	14,19,25,42	0
23	CLA	D	403	65/65	0.11	0.10	22,28,73,79	0
33	HTG	O	303	19/19	0.08	0.10	27,32,50,52	0
38	RRX	h	101	41/41	0.14	0.10	27,35,49,54	0
23	CLA	b	605	65/65	0.12	0.09	24,29,36,39	0
34	DGD	c	918	62/66	0.14	0.06	27,35,79,91	0
25	BCR	c	916	40/40	0.10	0.03	28,36,45,47	0
35	BCT	D	401	4/4	0.08	0.03	32,35,41,51	0
25	BCR	C	514	40/40	0.10	0.01	33,42,46,46	0
23	CLA	d	403	65/65	0.09	0.01	25,32,83,90	0
23	CLA	b	609	65/65	0.10	-0.02	23,31,57,63	0
35	BCT	a	408	4/4	0.08	-0.08	30,32,37,46	0
23	CLA	B	615	65/65	0.10	-0.08	19,24,67,74	0
23	CLA	c	906	65/65	0.10	-0.10	26,31,46,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	FE2	a	405	1/1	0.07	-0.15	27,27,27,27	0
25	BCR	k	101	40/40	0.10	-0.16	33,39,47,49	0
29	UNL	b	629	16/-	0.10	-0.16	43,48,56,60	0
32	CA	B	601	1/1	0.11	-0.18	81,81,81,81	0
25	BCR	K	102	40/40	0.08	-0.19	28,31,39,42	0
22	CL	a	407	1/1	0.11	-0.20	27,27,27,27	0
24	PHO	a	412	64/64	0.10	-0.22	17,22,26,27	0
23	CLA	B	607	65/65	0.09	-0.22	21,27,55,61	0
25	BCR	B	620	40/40	0.09	-0.24	22,31,41,44	0
33	HTG	B	624	19/19	0.08	-0.25	27,33,41,51	0
23	CLA	c	907	65/65	0.09	-0.34	28,36,76,80	0
37	HEM	V	201	43/43	0.07	-0.35	22,24,28,33	0
23	CLA	b	619	65/65	0.11	-0.41	25,32,89,97	0
23	CLA	C	507	65/65	0.09	-0.41	26,33,56,61	0
23	CLA	C	511	65/65	0.08	-0.43	27,34,40,42	0
23	CLA	c	912	65/65	0.09	-0.47	29,37,45,50	0
21	FE2	A	402	1/1	0.06	-0.47	26,26,26,26	0
37	HEM	F	101	43/43	0.11	-0.50	36,42,49,52	0
23	CLA	b	618	65/65	0.09	-0.53	24,30,49,53	0
25	BCR	a	415	40/40	0.08	-0.54	21,25,30,31	0
37	HEM	v	201	43/43	0.08	-0.65	25,31,35,38	0
31	GOL	B	634	6/6	0.10	-0.72	29,29,34,37	0
20	OEX	A	401	10/10	0.09	-0.73	21,23,27,28	0
39	MG	J	101	1/1	0.05	-0.83	28,28,28,28	0
20	OEX	a	404	10/10	0.09	-0.92	22,26,28,29	0
32	CA	f	103	1/1	0.18	-1.06	56,56,56,56	0
22	CL	A	404	1/1	0.12	-1.17	22,22,22,22	0
31	GOL	v	202	6/6	0.10	-1.45	35,36,40,41	0
32	CA	O	301	1/1	0.11	-1.53	49,49,49,49	0
22	CL	A	403	1/1	0.06	-1.82	25,25,25,25	0
32	CA	o	301	1/1	0.08	-1.91	51,51,51,51	0
32	CA	c	901	1/1	0.05	-3.55	46,46,46,46	0
22	CL	a	406	1/1	0.03	-4.53	29,29,29,29	0
31	GOL	h	103	6/6	0.33	-	78,83,83,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.