



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 06:49 AM GMT

PDB ID : 1QZV
Title : Crystal structure of plant photosystem I
Authors : Ben-Shem, A.; Frolow, F.; Nelson, N.
Deposited on : 2003-09-18
Resolution : 4.44 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>

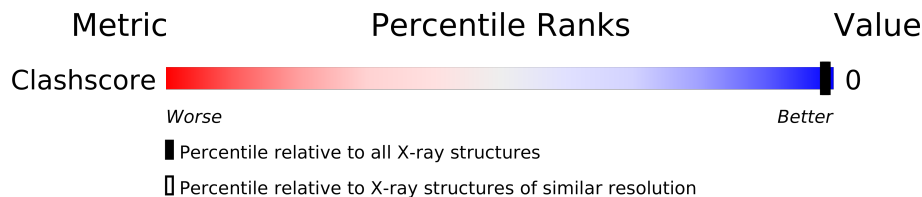
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 4.44 Å.



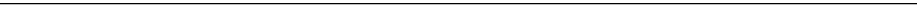
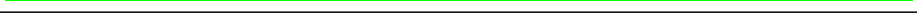




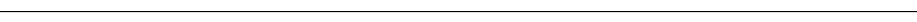








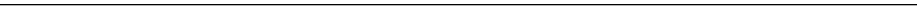


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1285 (5.30-3.50)










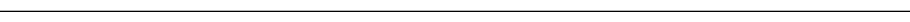

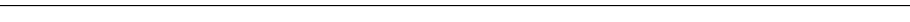
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	726	
1	P	726	
2	B	732	
2	Q	732	
3	C	80	
3	R	80	
4	D	154	
4	S	154	
5	E	64	
5	T	64	
6	F	154	
6	U	154	
7	G	74	
7	V	74	
8	H	52	
8	W	52	
9	I	30	
9	Y	30	
10	J	41	
10	Z	41	

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Mol	Chain	Length	Quality of chain
11	5	42	
11	K	42	
12	6	135	
12	L	135	
13	1	109	
13	7	109	
14	2	115	
14	8	115	
15	3	117	
15	9	117	
16	0	119	
16	4	119	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 13938 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 PLANT PHOTOSYSTEM I: SUBUNIT PSAA.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	726	Total	C	0	0	726
			726	726			
1	P	726	Total	C	0	0	726
			726	726			

- Molecule 2 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAB.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	732	Total	C	0	0	732
			732	732			
2	Q	732	Total	C	0	0	732
			732	732			

- Molecule 3 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAC.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	80	Total	C	0	0	80
			80	80			
3	R	80	Total	C	0	0	80
			80	80			

- Molecule 4 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAD.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	D	154	Total	C	0	0	154
			154	154			
4	S	154	Total	C	0	0	154
			154	154			

- Molecule 5 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	64	Total C 64 64	0	0	64
5	T	64	Total C 64 64	0	0	64

- Molecule 6 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAF.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	154	Total C 154 154	0	0	154
6	U	154	Total C 154 154	0	0	154

- Molecule 7 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAG.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	74	Total C 74 74	0	0	74
7	V	74	Total C 74 74	0	0	74

- Molecule 8 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAH.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	52	Total C 52 52	0	0	52
8	W	52	Total C 52 52	0	0	52

- Molecule 9 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAL.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	30	Total C 30 30	0	0	30
9	Y	30	Total C 30 30	0	0	30

- Molecule 10 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAJ.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	41	Total C 41 41	0	0	41

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	Z	41	Total C 41 41	0	0	41

- Molecule 11 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAK.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	K	42	Total C 42 42	0	0	42
11	5	42	Total C 42 42	0	0	42

- Molecule 12 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAL.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	L	135	Total C 135 135	0	0	135
12	6	135	Total C 135 135	0	0	135

- Molecule 13 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	1	109	Total C 109 109	0	0	109
13	7	109	Total C 109 109	0	0	109

- Molecule 14 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	2	115	Total C 115 115	0	0	115
14	8	115	Total C 115 115	0	0	115

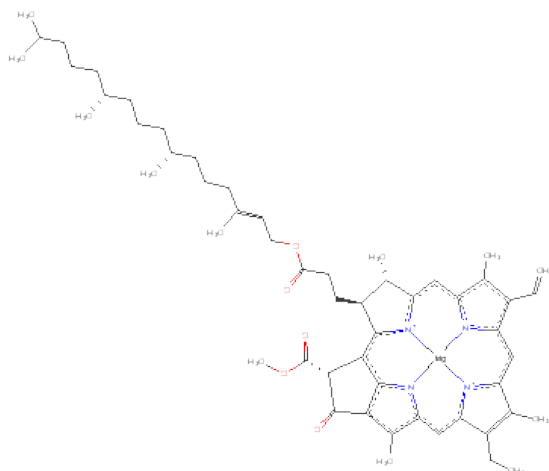
- Molecule 15 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
15	3	117	Total	C	0	0	117
			117	117			
15	9	117	Total	C	0	0	117
			117	117			

- Molecule 16 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
16	4	119	Total	C	0	0	119
			119	119			
16	0	119	Total	C	0	0	119
			119	119			

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	J	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	G	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	J	1	Total 25	C 20	Mg 1	N 4	0	0
17	K	1	Total 25	C 20	Mg 1	N 4	0	0
17	A	1	Total 25	C 20	Mg 1	N 4	0	0
17	K	1	Total 25	C 20	Mg 1	N 4	0	0
17	K	1	Total 25	C 20	Mg 1	N 4	0	0
17	L	1	Total 25	C 20	Mg 1	N 4	0	0
17	L	1	Total 25	C 20	Mg 1	N 4	0	0
17	L	1	Total 25	C 20	Mg 1	N 4	0	0
17	L	1	Total 25	C 20	Mg 1	N 4	0	0
17	G	1	Total 25	C 20	Mg 1	N 4	0	0
17	H	1	Total 25	C 20	Mg 1	N 4	0	0
17	A	1	Total 25	C 20	Mg 1	N 4	0	0
17	B	1	Total 25	C 20	Mg 1	N 4	0	0
17	4	1	Total 25	C 20	Mg 1	N 4	0	0
17	F	1	Total 25	C 20	Mg 1	N 4	0	0
17	F	1	Total 25	C 20	Mg 1	N 4	0	0
17	F	1	Total 25	C 20	Mg 1	N 4	0	0
17	F	1	Total 25	C 20	Mg 1	N 4	0	0
17	2	1	Total 25	C 20	Mg 1	N 4	0	0
17	J	1	Total 25	C 20	Mg 1	N 4	0	0
17	A	1	Total 25	C 20	Mg 1	N 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	V	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Z	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	V	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	W	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Z	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		

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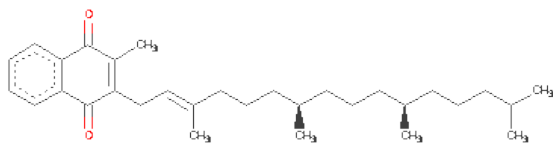
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		

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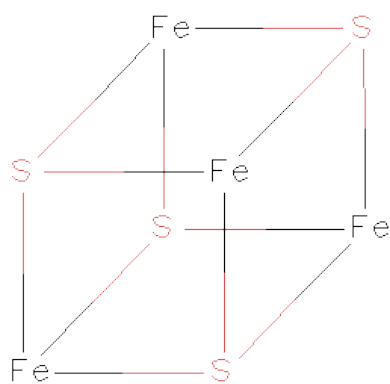
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			13	11	2		
18	B	1	Total	C	O	0	0
			13	11	2		
18	P	1	Total	C	O	0	0
			13	11	2		
18	Q	1	Total	C	O	0	0
			13	11	2		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total 8	Fe 4	S 4	0	0
19	C	1	Total 8	Fe 4	S 4	0	0
19	C	1	Total 8	Fe 4	S 4	0	0
19	P	1	Total 8	Fe 4	S 4	0	0
19	R	1	Total 8	Fe 4	S 4	0	0
19	R	1	Total 8	Fe 4	S 4	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.

Note EDS was not executed.

- Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain A: 

There are no outlier residues recorded for this chain.

- Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain P: 

There are no outlier residues recorded for this chain.

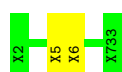
- Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain B: 



- Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain Q: 



- Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain C: 

There are no outlier residues recorded for this chain.

- Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain R: 

There are no outlier residues recorded for this chain.

- Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain D: 

There are no outlier residues recorded for this chain.

- Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain S: 

There are no outlier residues recorded for this chain.

- Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain E: 

There are no outlier residues recorded for this chain.

- Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain T: 

There are no outlier residues recorded for this chain.

- Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain F: 

There are no outlier residues recorded for this chain.

- Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain U: 

There are no outlier residues recorded for this chain.

- Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain G: 

There are no outlier residues recorded for this chain.

- Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain V: 

There are no outlier residues recorded for this chain.

- Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain H: 

There are no outlier residues recorded for this chain.

- Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain W: 

There are no outlier residues recorded for this chain.

- Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain I: 

There are no outlier residues recorded for this chain.

- Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain Y: 

There are no outlier residues recorded for this chain.

- Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain J: 

There are no outlier residues recorded for this chain.

- Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain Z: 

There are no outlier residues recorded for this chain.

- Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain K: 

There are no outlier residues recorded for this chain.

- Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain 5: 

There are no outlier residues recorded for this chain.

- Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain L: 

There are no outlier residues recorded for this chain.

- Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain 6: 

There are no outlier residues recorded for this chain.

- Molecule 13: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1

Chain 1: 

There are no outlier residues recorded for this chain.

- Molecule 13: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1

Chain 7: 

There are no outlier residues recorded for this chain.

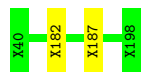
- Molecule 14: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2

Chain 2: 



- Molecule 14: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2

Chain 8: 



- Molecule 15: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA3

Chain 3: 

There are no outlier residues recorded for this chain.

- Molecule 15: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA3

Chain 9: 

There are no outlier residues recorded for this chain.

- Molecule 16: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA4

Chain 4: 

There are no outlier residues recorded for this chain.

- Molecule 16: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA4

Chain 0: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	182.28Å 190.38Å 220.25Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	50.00 – 4.44	Depositor
% Data completeness (in resolution range)	99.6 (50.00-4.44)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.410 , 0.420	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13938	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CLA, PQN

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	$\# Z > 5$

There are no bond length outliers.

There are no bond angle outliers.

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	726	0	0	0	0
1	P	726	0	0	0	0
2	B	732	0	0	1	0
2	Q	732	0	0	1	0
3	C	80	0	0	0	0
3	R	80	0	0	0	0
4	D	154	0	0	0	0
4	S	154	0	0	0	0
5	E	64	0	0	0	0
5	T	64	0	0	0	0
6	F	154	0	0	0	0
6	U	154	0	0	0	0
7	G	74	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	V	74	0	0	0	0
8	H	52	0	0	0	0
8	W	52	0	0	0	0
9	I	30	0	0	0	0
9	Y	30	0	0	0	0
10	J	41	0	0	0	0
10	Z	41	0	0	0	0
11	5	42	0	0	0	0
11	K	42	0	0	0	0
12	6	135	0	0	0	0
12	L	135	0	0	0	0
13	1	109	0	0	0	0
13	7	109	0	0	0	0
14	2	115	0	0	1	0
14	8	115	0	0	1	0
15	3	117	0	0	0	0
15	9	117	0	0	0	0
16	0	119	0	0	0	0
16	4	119	0	0	0	0
17	0	400	0	48	0	0
17	1	325	0	39	0	0
17	2	375	0	45	0	0
17	3	350	0	42	0	0
17	4	400	0	48	0	0
17	5	75	0	9	0	0
17	6	100	0	12	0	0
17	7	325	0	39	0	0
17	8	375	0	45	0	0
17	9	350	0	42	0	0
17	A	1125	0	135	0	0
17	B	1125	0	135	0	0
17	F	150	0	18	0	0
17	G	50	0	6	0	0
17	H	25	0	3	0	0
17	J	75	0	9	0	0
17	K	75	0	9	0	0
17	L	100	0	12	0	0
17	P	1125	0	135	0	0
17	Q	1125	0	135	0	0
17	U	150	0	18	0	0
17	V	50	0	6	0	0
17	W	25	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Z	75	0	9	0	0
18	A	13	0	7	0	0
18	B	13	0	7	0	0
18	P	13	0	7	0	0
18	Q	13	0	7	0	0
19	A	8	0	0	0	0
19	C	16	0	0	0	0
19	P	8	0	0	0	0
19	R	16	0	0	0	0
All	All	13938	0	1030	4	0

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 0.

All (4) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:8:182:UNK:CA	14:8:187:UNK:CA	2.92	0.48
14:2:182:UNK:CA	14:2:187:UNK:CA	2.92	0.47
2:B:5:UNK:CA	2:B:6:UNK:CA	2.97	0.42
2:Q:5:UNK:CA	2:Q:6:UNK:CA	2.97	0.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

344 ligands 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$
17	CLA	0	1011	-	23,32,73	21.00	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	0	1012	-	23,32,73	21.06	11 (47%)	12,54,113	1.82	3 (25%)
17	CLA	0	1013	-	23,32,73	20.97	10 (43%)	12,54,113	1.79	2 (16%)
17	CLA	0	1014	-	23,32,73	20.90	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	0	1015	-	23,32,73	21.13	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	0	1016	-	23,32,73	21.10	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	0	1017	-	23,32,73	20.91	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	0	1021	-	23,32,73	21.03	11 (47%)	12,54,113	1.77	2 (16%)
17	CLA	0	1022	-	23,32,73	21.22	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	0	1023	-	23,32,73	20.77	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	0	1025	-	23,32,73	20.87	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	0	1026	-	23,32,73	21.02	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	0	1031	-	23,32,73	21.00	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	0	1032	-	23,32,73	21.02	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	0	1033	-	23,32,73	20.97	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	0	8002	-	23,32,73	21.03	12 (52%)	12,54,113	1.83	2 (16%)
17	CLA	1	1011	-	23,32,73	21.00	12 (52%)	12,54,113	1.82	2 (16%)
17	CLA	1	1012	-	23,32,73	20.92	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	1	1013	-	23,32,73	20.96	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	1	1014	-	23,32,73	20.95	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1015	-	23,32,73	20.87	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1016	-	23,32,73	20.94	11 (47%)	12,54,113	1.79	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	1	1017	-	23,32,73	21.01	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1021	-	23,32,73	21.00	12 (52%)	12,54,113	1.79	2 (16%)
17	CLA	1	1022	-	23,32,73	20.84	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1023	-	23,32,73	21.11	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	1	1025	-	23,32,73	20.95	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1026	-	23,32,73	20.72	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1031	-	23,32,73	20.85	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	2	1011	-	23,32,73	20.99	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	2	1012	-	23,32,73	20.87	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	2	1013	-	23,32,73	20.93	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	2	1014	-	23,32,73	20.81	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	2	1015	-	23,32,73	20.87	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	2	1016	-	23,32,73	20.86	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	2	1017	-	23,32,73	21.21	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	2	1021	-	23,32,73	20.83	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	2	1022	-	23,32,73	21.09	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	2	1023	-	23,32,73	20.94	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	2	1025	-	23,32,73	20.98	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	2	1026	-	23,32,73	20.91	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	2	1031	-	23,32,73	20.95	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	2	1033	-	23,32,73	21.01	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	2	4007	-	23,32,73	20.97	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1011	-	23,32,73	21.00	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	3	1012	-	23,32,73	20.91	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	3	1014	-	23,32,73	20.92	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	3	1015	-	23,32,73	20.95	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1016	-	23,32,73	20.94	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	3	1017	-	23,32,73	20.95	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1021	-	23,32,73	21.00	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1022	-	23,32,73	20.89	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	3	1025	-	23,32,73	20.77	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1026	-	23,32,73	20.94	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1031	-	23,32,73	20.91	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1032	-	23,32,73	21.08	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	3	1033	-	23,32,73	20.91	11 (47%)	12,54,113	1.82	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	3	1041	-	23,32,73	20.97	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1011	-	23,32,73	21.10	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	4	1012	-	23,32,73	21.17	11 (47%)	12,54,113	1.83	3 (25%)
17	CLA	4	1013	-	23,32,73	21.01	10 (43%)	12,54,113	1.80	2 (16%)
17	CLA	4	1014	-	23,32,73	20.88	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	4	1015	-	23,32,73	21.14	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1016	-	23,32,73	21.00	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1017	-	23,32,73	20.82	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	4	1021	-	23,32,73	20.99	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	4	1022	-	23,32,73	21.09	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1023	-	23,32,73	20.86	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	4	1025	-	23,32,73	20.89	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	4	1026	-	23,32,73	21.06	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1031	-	23,32,73	21.04	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	4	1032	-	23,32,73	21.00	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1033	-	23,32,73	21.07	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	4002	-	23,32,73	21.00	12 (52%)	12,54,113	1.82	2 (16%)
17	CLA	5	5401	-	23,32,73	20.98	11 (47%)	12,54,113	1.63	2 (16%)
17	CLA	5	5403	-	23,32,73	21.06	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	5	5404	-	23,32,73	21.11	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	6	5501	-	23,32,73	22.22	10 (43%)	12,54,113	1.60	2 (16%)
17	CLA	6	5502	-	23,32,73	20.90	10 (43%)	12,54,113	1.74	2 (16%)
17	CLA	6	5503	-	23,32,73	19.82	9 (39%)	12,54,113	1.62	2 (16%)
17	CLA	6	5504	-	23,32,73	20.92	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	7	1011	-	23,32,73	21.00	12 (52%)	12,54,113	1.82	2 (16%)
17	CLA	7	1012	-	23,32,73	20.97	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	7	1013	-	23,32,73	20.95	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	7	1014	-	23,32,73	20.89	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	7	1015	-	23,32,73	20.83	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	7	1016	-	23,32,73	20.89	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	7	1017	-	23,32,73	21.05	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	7	1021	-	23,32,73	20.97	12 (52%)	12,54,113	1.79	2 (16%)
17	CLA	7	1022	-	23,32,73	20.88	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	7	1023	-	23,32,73	20.98	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	7	1025	-	23,32,73	20.97	11 (47%)	12,54,113	1.81	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	7	1026	-	23,32,73	20.71	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	7	1031	-	23,32,73	20.93	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	8	1011	-	23,32,73	21.04	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	8	1012	-	23,32,73	20.84	12 (52%)	12,54,113	1.82	2 (16%)
17	CLA	8	1013	-	23,32,73	20.91	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	8	1014	-	23,32,73	20.83	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	8	1015	-	23,32,73	20.90	12 (52%)	12,54,113	1.80	2 (16%)
17	CLA	8	1016	-	23,32,73	20.93	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	8	1017	-	23,32,73	21.13	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	8	1021	-	23,32,73	20.88	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	8	1022	-	23,32,73	21.09	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	8	1023	-	23,32,73	20.95	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	8	1025	-	23,32,73	21.07	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	8	1026	-	23,32,73	20.92	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	8	1031	-	23,32,73	20.90	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	8	1033	-	23,32,73	21.08	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	8	8007	-	23,32,73	20.93	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	9	1011	-	23,32,73	21.06	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	9	1012	-	23,32,73	20.79	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	9	1014	-	23,32,73	20.91	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	9	1015	-	23,32,73	20.90	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	9	1016	-	23,32,73	20.93	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	9	1017	-	23,32,73	20.91	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	9	1021	-	23,32,73	20.96	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	9	1022	-	23,32,73	20.86	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	9	1025	-	23,32,73	20.73	10 (43%)	12,54,113	1.80	2 (16%)
17	CLA	9	1026	-	23,32,73	21.02	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	9	1031	-	23,32,73	20.96	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	9	1032	-	23,32,73	21.08	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	9	1033	-	23,32,73	21.05	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	9	1041	-	23,32,73	20.97	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	A	1011	-	23,32,73	20.99	9 (39%)	12,54,113	1.62	1 (8%)
17	CLA	A	1012	-	23,32,73	19.06	10 (43%)	12,54,113	1.78	3 (25%)
17	CLA	A	1013	-	23,32,73	20.55	12 (52%)	12,54,113	1.54	2 (16%)
17	CLA	A	1102	-	23,32,73	18.40	10 (43%)	12,54,113	1.68	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	1103	-	23,32,73	19.31	11 (47%)	12,54,113	1.92	2 (16%)
17	CLA	A	1104	-	23,32,73	20.57	10 (43%)	12,54,113	1.72	2 (16%)
17	CLA	A	1105	-	23,32,73	20.20	10 (43%)	12,54,113	1.56	1 (8%)
17	CLA	A	1106	-	23,32,73	20.10	11 (47%)	12,54,113	1.77	3 (25%)
17	CLA	A	1107	-	23,32,73	18.31	10 (43%)	12,54,113	1.72	1 (8%)
17	CLA	A	1108	-	23,32,73	18.46	11 (47%)	12,54,113	2.42	6 (50%)
17	CLA	A	1109	-	23,32,73	20.16	11 (47%)	12,54,113	1.64	2 (16%)
17	CLA	A	1110	-	23,32,73	21.30	10 (43%)	12,54,113	1.83	2 (16%)
17	CLA	A	1111	-	23,32,73	21.45	11 (47%)	12,54,113	1.86	3 (25%)
17	CLA	A	1112	-	23,32,73	22.18	12 (52%)	12,54,113	1.65	2 (16%)
17	CLA	A	1113	-	23,32,73	19.93	12 (52%)	12,54,113	2.63	5 (41%)
17	CLA	A	1114	-	23,32,73	19.70	11 (47%)	12,54,113	1.69	2 (16%)
17	CLA	A	1115	-	23,32,73	21.67	10 (43%)	12,54,113	1.51	1 (8%)
17	CLA	A	1116	-	23,32,73	19.94	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	A	1117	-	23,32,73	17.11	9 (39%)	12,54,113	1.62	2 (16%)
17	CLA	A	1118	-	23,32,73	22.19	10 (43%)	12,54,113	1.89	3 (25%)
17	CLA	A	1119	-	23,32,73	18.96	11 (47%)	12,54,113	1.72	2 (16%)
17	CLA	A	1120	-	23,32,73	20.55	10 (43%)	12,54,113	1.74	2 (16%)
17	CLA	A	1121	-	23,32,73	20.36	12 (52%)	12,54,113	1.51	2 (16%)
17	CLA	A	1122	-	23,32,73	18.64	12 (52%)	12,54,113	1.70	2 (16%)
17	CLA	A	1123	-	23,32,73	21.12	10 (43%)	12,54,113	1.79	2 (16%)
17	CLA	A	1124	-	23,32,73	18.53	10 (43%)	12,54,113	1.62	2 (16%)
17	CLA	A	1125	-	23,32,73	22.07	10 (43%)	12,54,113	1.87	3 (25%)
17	CLA	A	1126	-	23,32,73	20.20	10 (43%)	12,54,113	1.63	2 (16%)
17	CLA	A	1127	-	23,32,73	17.68	11 (47%)	12,54,113	1.62	1 (8%)
17	CLA	A	1128	-	23,32,73	22.26	10 (43%)	12,54,113	1.60	2 (16%)
17	CLA	A	1129	-	23,32,73	20.30	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	A	1131	-	23,32,73	17.18	11 (47%)	12,54,113	1.68	2 (16%)
17	CLA	A	1132	-	23,32,73	16.86	10 (43%)	12,54,113	1.68	2 (16%)
17	CLA	A	1133	-	23,32,73	18.64	10 (43%)	12,54,113	1.74	2 (16%)
17	CLA	A	1134	-	23,32,73	21.35	10 (43%)	12,54,113	1.78	2 (16%)
17	CLA	A	1135	-	23,32,73	21.15	9 (39%)	12,54,113	1.77	2 (16%)
17	CLA	A	1136	-	23,32,73	23.08	11 (47%)	12,54,113	1.59	2 (16%)
17	CLA	A	1137	-	23,32,73	20.60	12 (52%)	12,54,113	2.43	5 (41%)
17	CLA	A	1138	-	23,32,73	21.46	10 (43%)	12,54,113	1.79	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	1139	-	23,32,73	18.64	9 (39%)	12,54,113	1.59	1 (8%)
17	CLA	A	1140	-	23,32,73	20.86	10 (43%)	12,54,113	1.78	2 (16%)
17	CLA	A	1402	-	23,32,73	21.14	9 (39%)	12,54,113	1.80	2 (16%)
17	CLA	A	1901	-	23,32,73	20.66	12 (52%)	12,54,113	2.77	5 (41%)
18	PQN	A	2001	-	12,14,34	6.26	8 (66%)	15,20,45	0.70	0
19	SF4	A	3001	-	12,12,12	7.84	12 (100%)	0,24,24	0.00	-
17	CLA	A	4009	-	23,32,73	20.89	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	A	4010	-	23,32,73	21.00	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	B	1021	-	23,32,73	19.22	10 (43%)	12,54,113	1.66	2 (16%)
17	CLA	B	1022	-	23,32,73	19.72	11 (47%)	12,54,113	1.80	3 (25%)
17	CLA	B	1023	-	23,32,73	23.86	13 (56%)	12,54,113	1.73	2 (16%)
17	CLA	B	1130	-	23,32,73	21.55	10 (43%)	12,54,113	1.78	2 (16%)
17	CLA	B	1201	-	23,32,73	19.93	9 (39%)	12,54,113	1.75	3 (25%)
17	CLA	B	1202	-	23,32,73	18.97	8 (34%)	12,54,113	1.78	2 (16%)
17	CLA	B	1203	-	23,32,73	20.90	9 (39%)	12,54,113	1.71	2 (16%)
17	CLA	B	1204	-	23,32,73	21.17	11 (47%)	12,54,113	1.85	2 (16%)
17	CLA	B	1205	-	23,32,73	21.40	11 (47%)	12,54,113	1.55	1 (8%)
17	CLA	B	1206	-	23,32,73	15.62	8 (34%)	12,54,113	1.77	1 (8%)
17	CLA	B	1207	-	23,32,73	21.70	9 (39%)	12,54,113	1.72	2 (16%)
17	CLA	B	1208	-	23,32,73	20.35	11 (47%)	12,54,113	1.66	2 (16%)
17	CLA	B	1209	-	23,32,73	21.78	11 (47%)	12,54,113	1.71	2 (16%)
17	CLA	B	1210	-	23,32,73	21.00	12 (52%)	12,54,113	1.79	2 (16%)
17	CLA	B	1211	-	23,32,73	18.88	11 (47%)	12,54,113	1.65	2 (16%)
17	CLA	B	1212	-	23,32,73	21.03	11 (47%)	12,54,113	1.63	1 (8%)
17	CLA	B	1213	-	23,32,73	21.22	11 (47%)	12,54,113	1.60	2 (16%)
17	CLA	B	1214	-	23,32,73	20.35	11 (47%)	12,54,113	1.70	2 (16%)
17	CLA	B	1215	-	23,32,73	18.07	9 (39%)	12,54,113	1.72	2 (16%)
17	CLA	B	1216	-	23,32,73	19.35	12 (52%)	12,54,113	1.59	2 (16%)
17	CLA	B	1217	-	23,32,73	20.45	10 (43%)	12,54,113	1.76	2 (16%)
17	CLA	B	1218	-	23,32,73	21.63	10 (43%)	12,54,113	1.77	2 (16%)
17	CLA	B	1219	-	23,32,73	22.30	12 (52%)	12,54,113	2.52	4 (33%)
17	CLA	B	1220	-	23,32,73	21.13	9 (39%)	12,54,113	1.69	2 (16%)
17	CLA	B	1221	-	23,32,73	21.65	11 (47%)	12,54,113	1.90	3 (25%)
17	CLA	B	1222	-	23,32,73	19.22	9 (39%)	12,54,113	1.68	2 (16%)
17	CLA	B	1223	-	23,32,73	20.97	11 (47%)	12,54,113	1.82	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	1224	-	23,32,73	20.87	10 (43%)	12,54,113	1.74	2 (16%)
17	CLA	B	1225	-	23,32,73	18.23	10 (43%)	12,54,113	1.40	1 (8%)
17	CLA	B	1226	-	23,32,73	18.91	11 (47%)	12,54,113	1.58	2 (16%)
17	CLA	B	1227	-	23,32,73	19.68	12 (52%)	12,54,113	1.74	2 (16%)
17	CLA	B	1228	-	23,32,73	21.38	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	B	1230	-	23,32,73	20.32	11 (47%)	12,54,113	1.66	2 (16%)
17	CLA	B	1231	-	23,32,73	22.48	11 (47%)	12,54,113	1.83	2 (16%)
17	CLA	B	1232	-	23,32,73	21.88	11 (47%)	12,54,113	1.68	2 (16%)
17	CLA	B	1234	-	23,32,73	21.07	9 (39%)	12,54,113	1.72	2 (16%)
17	CLA	B	1235	-	23,32,73	21.26	11 (47%)	12,54,113	1.70	2 (16%)
17	CLA	B	1236	-	23,32,73	18.39	11 (47%)	12,54,113	1.60	2 (16%)
17	CLA	B	1237	-	23,32,73	18.51	9 (39%)	12,54,113	1.74	2 (16%)
17	CLA	B	1238	-	23,32,73	18.13	9 (39%)	12,54,113	1.58	1 (8%)
17	CLA	B	1239	-	23,32,73	17.34	9 (39%)	12,54,113	1.71	2 (16%)
17	CLA	B	1240	-	23,32,73	20.90	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	B	1241	-	23,32,73	20.95	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	B	1242	-	23,32,73	21.02	11 (47%)	12,54,113	1.79	2 (16%)
18	PQN	B	2002	-	12,14,34	6.05	8 (66%)	15,20,45	0.80	0
17	CLA	B	4001	-	23,32,73	20.94	11 (47%)	12,54,113	1.81	2 (16%)
19	SF4	C	3002	-	12,12,12	10.20	10 (83%)	0,24,24	0.00	-
19	SF4	C	3003	-	12,12,12	5.85	11 (91%)	0,24,24	0.00	-
17	CLA	F	1229	-	23,32,73	20.37	10 (43%)	12,54,113	1.72	2 (16%)
17	CLA	F	1301	-	23,32,73	21.93	11 (47%)	12,54,113	1.62	1 (8%)
17	CLA	F	4003	-	23,32,73	20.72	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	F	4004	-	23,32,73	20.97	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	F	4005	-	23,32,73	20.93	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	F	4006	-	23,32,73	20.97	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	G	1233	-	23,32,73	21.03	10 (43%)	12,54,113	1.72	2 (16%)
17	CLA	G	1701	-	23,32,73	20.98	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	H	1801	-	23,32,73	21.03	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	J	1101	-	23,32,73	20.96	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	J	1302	-	23,32,73	20.11	12 (52%)	12,54,113	2.70	6 (50%)
17	CLA	J	4008	-	23,32,73	20.98	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	K	1401	-	23,32,73	21.04	11 (47%)	12,54,113	1.64	2 (16%)
17	CLA	K	1403	-	23,32,73	21.03	11 (47%)	12,54,113	1.80	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	K	1404	-	23,32,73	21.10	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	L	1501	-	23,32,73	22.13	10 (43%)	12,54,113	1.59	2 (16%)
17	CLA	L	1502	-	23,32,73	20.90	10 (43%)	12,54,113	1.72	2 (16%)
17	CLA	L	1503	-	23,32,73	19.73	10 (43%)	12,54,113	1.62	2 (16%)
17	CLA	L	1504	-	23,32,73	20.89	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	P	5011	-	23,32,73	21.12	9 (39%)	12,54,113	1.62	1 (8%)
17	CLA	P	5012	-	23,32,73	19.10	10 (43%)	12,54,113	1.77	3 (25%)
17	CLA	P	5013	-	23,32,73	20.63	12 (52%)	12,54,113	1.54	2 (16%)
17	CLA	P	5102	-	23,32,73	18.40	10 (43%)	12,54,113	1.67	2 (16%)
17	CLA	P	5103	-	23,32,73	19.30	11 (47%)	12,54,113	1.92	2 (16%)
17	CLA	P	5104	-	23,32,73	20.59	10 (43%)	12,54,113	1.72	2 (16%)
17	CLA	P	5105	-	23,32,73	20.22	10 (43%)	12,54,113	1.56	1 (8%)
17	CLA	P	5106	-	23,32,73	20.09	11 (47%)	12,54,113	1.77	3 (25%)
17	CLA	P	5107	-	23,32,73	18.53	10 (43%)	12,54,113	1.71	1 (8%)
17	CLA	P	5108	-	23,32,73	18.52	10 (43%)	12,54,113	2.42	6 (50%)
17	CLA	P	5109	-	23,32,73	20.13	11 (47%)	12,54,113	1.65	2 (16%)
17	CLA	P	5110	-	23,32,73	21.23	10 (43%)	12,54,113	1.84	3 (25%)
17	CLA	P	5111	-	23,32,73	21.54	11 (47%)	12,54,113	1.86	3 (25%)
17	CLA	P	5112	-	23,32,73	22.22	12 (52%)	12,54,113	1.64	2 (16%)
17	CLA	P	5113	-	23,32,73	20.06	12 (52%)	12,54,113	2.63	5 (41%)
17	CLA	P	5114	-	23,32,73	19.72	11 (47%)	12,54,113	1.69	2 (16%)
17	CLA	P	5115	-	23,32,73	21.68	10 (43%)	12,54,113	1.51	1 (8%)
17	CLA	P	5116	-	23,32,73	19.87	10 (43%)	12,54,113	1.79	2 (16%)
17	CLA	P	5117	-	23,32,73	17.11	9 (39%)	12,54,113	1.62	1 (8%)
17	CLA	P	5118	-	23,32,73	22.14	10 (43%)	12,54,113	1.89	3 (25%)
17	CLA	P	5119	-	23,32,73	18.97	12 (52%)	12,54,113	1.72	2 (16%)
17	CLA	P	5120	-	23,32,73	20.54	10 (43%)	12,54,113	1.74	2 (16%)
17	CLA	P	5121	-	23,32,73	20.36	12 (52%)	12,54,113	1.52	2 (16%)
17	CLA	P	5122	-	23,32,73	18.73	12 (52%)	12,54,113	1.71	2 (16%)
17	CLA	P	5123	-	23,32,73	21.08	10 (43%)	12,54,113	1.80	2 (16%)
17	CLA	P	5124	-	23,32,73	18.46	10 (43%)	12,54,113	1.64	2 (16%)
17	CLA	P	5125	-	23,32,73	22.14	10 (43%)	12,54,113	1.87	3 (25%)
17	CLA	P	5126	-	23,32,73	20.23	11 (47%)	12,54,113	1.63	2 (16%)
17	CLA	P	5127	-	23,32,73	17.71	10 (43%)	12,54,113	1.62	1 (8%)
17	CLA	P	5128	-	23,32,73	22.35	10 (43%)	12,54,113	1.61	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	P	5129	-	23,32,73	20.39	10 (43%)	12,54,113	1.81	2 (16%)
17	CLA	P	5131	-	23,32,73	17.24	11 (47%)	12,54,113	1.67	2 (16%)
17	CLA	P	5132	-	23,32,73	16.79	10 (43%)	12,54,113	1.67	2 (16%)
17	CLA	P	5133	-	23,32,73	18.67	10 (43%)	12,54,113	1.73	2 (16%)
17	CLA	P	5134	-	23,32,73	21.36	10 (43%)	12,54,113	1.78	2 (16%)
17	CLA	P	5135	-	23,32,73	21.20	9 (39%)	12,54,113	1.75	2 (16%)
17	CLA	P	5136	-	23,32,73	23.15	11 (47%)	12,54,113	1.59	2 (16%)
17	CLA	P	5137	-	23,32,73	20.73	12 (52%)	12,54,113	2.44	5 (41%)
17	CLA	P	5138	-	23,32,73	21.45	10 (43%)	12,54,113	1.80	3 (25%)
17	CLA	P	5139	-	23,32,73	18.59	9 (39%)	12,54,113	1.59	1 (8%)
17	CLA	P	5140	-	23,32,73	20.82	10 (43%)	12,54,113	1.78	2 (16%)
17	CLA	P	5402	-	23,32,73	21.22	9 (39%)	12,54,113	1.80	2 (16%)
17	CLA	P	5901	-	23,32,73	20.70	12 (52%)	12,54,113	2.76	5 (41%)
18	PQN	P	6001	-	12,14,34	6.26	9 (75%)	15,20,45	0.70	0
19	SF4	P	7001	-	12,12,12	7.86	12 (100%)	0,24,24	0.00	-
17	CLA	P	8009	-	23,32,73	20.83	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	P	8010	-	23,32,73	20.98	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	Q	5021	-	23,32,73	19.29	10 (43%)	12,54,113	1.65	2 (16%)
17	CLA	Q	5022	-	23,32,73	19.71	11 (47%)	12,54,113	1.79	3 (25%)
17	CLA	Q	5023	-	23,32,73	23.84	13 (56%)	12,54,113	1.74	2 (16%)
17	CLA	Q	5130	-	23,32,73	21.61	10 (43%)	12,54,113	1.79	2 (16%)
17	CLA	Q	5201	-	23,32,73	19.84	9 (39%)	12,54,113	1.75	3 (25%)
17	CLA	Q	5202	-	23,32,73	19.06	8 (34%)	12,54,113	1.78	2 (16%)
17	CLA	Q	5203	-	23,32,73	21.09	9 (39%)	12,54,113	1.73	2 (16%)
17	CLA	Q	5204	-	23,32,73	21.13	11 (47%)	12,54,113	1.85	2 (16%)
17	CLA	Q	5205	-	23,32,73	21.34	11 (47%)	12,54,113	1.56	1 (8%)
17	CLA	Q	5206	-	23,32,73	15.64	8 (34%)	12,54,113	1.77	1 (8%)
17	CLA	Q	5207	-	23,32,73	21.69	9 (39%)	12,54,113	1.73	2 (16%)
17	CLA	Q	5208	-	23,32,73	20.25	11 (47%)	12,54,113	1.65	2 (16%)
17	CLA	Q	5209	-	23,32,73	21.71	11 (47%)	12,54,113	1.70	2 (16%)
17	CLA	Q	5210	-	23,32,73	20.97	12 (52%)	12,54,113	1.78	2 (16%)
17	CLA	Q	5211	-	23,32,73	18.81	11 (47%)	12,54,113	1.66	2 (16%)
17	CLA	Q	5212	-	23,32,73	21.06	11 (47%)	12,54,113	1.64	1 (8%)
17	CLA	Q	5213	-	23,32,73	21.29	11 (47%)	12,54,113	1.60	2 (16%)
17	CLA	Q	5214	-	23,32,73	20.45	10 (43%)	12,54,113	1.71	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	Q	5215	-	23,32,73	17.98	9 (39%)	12,54,113	1.73	2 (16%)
17	CLA	Q	5216	-	23,32,73	19.35	12 (52%)	12,54,113	1.59	2 (16%)
17	CLA	Q	5217	-	23,32,73	20.50	10 (43%)	12,54,113	1.76	2 (16%)
17	CLA	Q	5218	-	23,32,73	21.61	10 (43%)	12,54,113	1.76	2 (16%)
17	CLA	Q	5219	-	23,32,73	22.25	12 (52%)	12,54,113	2.52	4 (33%)
17	CLA	Q	5220	-	23,32,73	21.18	9 (39%)	12,54,113	1.70	2 (16%)
17	CLA	Q	5221	-	23,32,73	21.57	11 (47%)	12,54,113	1.90	3 (25%)
17	CLA	Q	5222	-	23,32,73	19.26	10 (43%)	12,54,113	1.68	2 (16%)
17	CLA	Q	5223	-	23,32,73	20.98	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	Q	5224	-	23,32,73	20.91	10 (43%)	12,54,113	1.73	2 (16%)
17	CLA	Q	5225	-	23,32,73	18.29	10 (43%)	12,54,113	1.41	1 (8%)
17	CLA	Q	5226	-	23,32,73	18.93	10 (43%)	12,54,113	1.57	2 (16%)
17	CLA	Q	5227	-	23,32,73	19.77	12 (52%)	12,54,113	1.74	2 (16%)
17	CLA	Q	5228	-	23,32,73	21.50	11 (47%)	12,54,113	1.83	2 (16%)
17	CLA	Q	5230	-	23,32,73	20.30	11 (47%)	12,54,113	1.66	2 (16%)
17	CLA	Q	5231	-	23,32,73	22.37	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	Q	5232	-	23,32,73	21.76	11 (47%)	12,54,113	1.67	2 (16%)
17	CLA	Q	5234	-	23,32,73	21.04	9 (39%)	12,54,113	1.71	2 (16%)
17	CLA	Q	5235	-	23,32,73	21.21	11 (47%)	12,54,113	1.70	2 (16%)
17	CLA	Q	5236	-	23,32,73	18.30	11 (47%)	12,54,113	1.61	2 (16%)
17	CLA	Q	5237	-	23,32,73	18.49	9 (39%)	12,54,113	1.75	2 (16%)
17	CLA	Q	5238	-	23,32,73	18.09	9 (39%)	12,54,113	1.59	2 (16%)
17	CLA	Q	5239	-	23,32,73	17.32	9 (39%)	12,54,113	1.71	2 (16%)
17	CLA	Q	5240	-	23,32,73	20.84	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	Q	5241	-	23,32,73	20.90	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	Q	5242	-	23,32,73	21.04	11 (47%)	12,54,113	1.79	2 (16%)
18	PQN	Q	6002	-	12,14,34	6.06	7 (58%)	15,20,45	0.80	0
17	CLA	Q	8001	-	23,32,73	20.89	11 (47%)	12,54,113	1.81	2 (16%)
19	SF4	R	7002	-	12,12,12	10.16	10 (83%)	0,24,24	0.00	-
19	SF4	R	7003	-	12,12,12	5.84	11 (91%)	0,24,24	0.00	-
17	CLA	U	5229	-	23,32,73	20.40	10 (43%)	12,54,113	1.73	2 (16%)
17	CLA	U	5301	-	23,32,73	21.82	11 (47%)	12,54,113	1.62	1 (8%)
17	CLA	U	8003	-	23,32,73	20.62	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	U	8004	-	23,32,73	20.96	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	U	8005	-	23,32,73	21.02	11 (47%)	12,54,113	1.81	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	U	8006	-	23,32,73	20.87	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	V	5233	-	23,32,73	21.06	10 (43%)	12,54,113	1.71	2 (16%)
17	CLA	V	5701	-	23,32,73	21.01	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	W	5801	-	23,32,73	21.06	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	Z	5101	-	23,32,73	20.95	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	Z	5302	-	23,32,73	20.10	12 (52%)	12,54,113	2.70	5 (41%)
17	CLA	Z	8008	-	23,32,73	21.07	11 (47%)	12,54,113	1.81	2 (16%)

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
17	CLA	0	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1032	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	0	8002	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1025	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	2	4007	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1032	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1041	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1025	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	4	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1032	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	4	4002	-	-	0/0/66/135	0/0/8/9
17	CLA	5	5401	-	-	0/0/66/135	0/0/8/9
17	CLA	5	5403	-	-	0/0/66/135	0/0/8/9
17	CLA	5	5404	-	-	0/0/66/135	0/0/8/9
17	CLA	6	5501	-	-	0/0/66/135	0/0/8/9
17	CLA	6	5502	-	-	0/0/66/135	0/0/8/9
17	CLA	6	5503	-	-	0/0/66/135	0/0/8/9
17	CLA	6	5504	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	8	8007	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1012	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	9	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1032	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1041	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1102	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1103	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1104	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1105	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1106	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1107	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1108	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1109	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1110	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1111	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1112	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1113	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1114	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1115	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1116	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1117	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1118	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1119	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1120	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1121	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1122	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1123	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1124	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1125	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1126	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1127	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1128	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	1129	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1131	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1132	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1133	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1134	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1135	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1136	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1137	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1138	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1139	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1140	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1402	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1901	-	-	0/0/66/135	0/0/8/9
18	PQN	A	2001	-	-	0/0/16/43	0/0/2/2
19	SF4	A	3001	-	-	0/0/48/48	0/0/5/5
17	CLA	A	4009	-	-	0/0/66/135	0/0/8/9
17	CLA	A	4010	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1130	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1201	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1202	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1203	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1204	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1205	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1206	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1207	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1208	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1209	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1210	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1211	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1212	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1213	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1214	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1215	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1216	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1217	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1218	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1219	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1220	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1221	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	1222	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1223	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1224	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1225	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1226	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1227	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1228	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1230	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1231	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1232	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1234	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1235	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1236	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1237	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1238	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1239	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1240	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1241	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1242	-	-	0/0/66/135	0/0/8/9
18	PQN	B	2002	-	-	0/0/16/43	0/0/2/2
17	CLA	B	4001	-	-	0/0/66/135	0/0/8/9
19	SF4	C	3002	-	-	0/0/48/48	0/0/5/5
19	SF4	C	3003	-	-	0/0/48/48	0/0/5/5
17	CLA	F	1229	-	-	0/0/66/135	0/0/8/9
17	CLA	F	1301	-	-	0/0/66/135	0/0/8/9
17	CLA	F	4003	-	-	0/0/66/135	0/0/8/9
17	CLA	F	4004	-	-	0/0/66/135	0/0/8/9
17	CLA	F	4005	-	-	0/0/66/135	0/0/8/9
17	CLA	F	4006	-	-	0/0/66/135	0/0/8/9
17	CLA	G	1233	-	-	0/0/66/135	0/0/8/9
17	CLA	G	1701	-	-	0/0/66/135	0/0/8/9
17	CLA	H	1801	-	-	0/0/66/135	0/0/8/9
17	CLA	J	1101	-	-	0/0/66/135	0/0/8/9
17	CLA	J	1302	-	-	0/0/66/135	0/0/8/9
17	CLA	J	4008	-	-	0/0/66/135	0/0/8/9
17	CLA	K	1401	-	-	0/0/66/135	0/0/8/9
17	CLA	K	1403	-	-	0/0/66/135	0/0/8/9
17	CLA	K	1404	-	-	0/0/66/135	0/0/8/9
17	CLA	L	1501	-	-	0/0/66/135	0/0/8/9
17	CLA	L	1502	-	-	0/0/66/135	0/0/8/9
17	CLA	L	1503	-	-	0/0/66/135	0/0/8/9
17	CLA	L	1504	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	P	5011	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5012	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5013	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5102	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5103	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5104	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5105	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5106	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5107	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5108	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5109	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5110	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5111	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5112	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5113	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5114	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5115	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5116	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5117	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5118	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5119	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5120	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5121	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5122	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5123	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5124	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5125	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5126	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5127	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5128	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5129	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5131	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5132	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5133	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5134	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5135	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5136	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5137	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5138	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5139	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5140	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5402	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	P	5901	-	-	0/0/66/135	0/0/8/9
18	PQN	P	6001	-	-	0/0/16/43	0/0/2/2
19	SF4	P	7001	-	-	0/0/48/48	0/0/5/5
17	CLA	P	8009	-	-	0/0/66/135	0/0/8/9
17	CLA	P	8010	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5021	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5022	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5023	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5130	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5201	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5202	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5203	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5204	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5205	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5206	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5207	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5208	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5209	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5210	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5211	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5212	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5213	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5214	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5215	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5216	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5217	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5218	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5219	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5220	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5221	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5222	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5223	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5224	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5225	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5226	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5227	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5228	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5230	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5231	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5232	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5234	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5235	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	Q	5236	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5237	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5238	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5239	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5240	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5241	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5242	-	-	0/0/66/135	0/0/8/9
18	PQN	Q	6002	-	-	0/0/16/43	0/0/2/2
17	CLA	Q	8001	-	-	0/0/66/135	0/0/8/9
19	SF4	R	7002	-	-	0/0/48/48	0/0/5/5
19	SF4	R	7003	-	-	0/0/48/48	0/0/5/5
17	CLA	U	5229	-	-	0/0/66/135	0/0/8/9
17	CLA	U	5301	-	-	0/0/66/135	0/0/8/9
17	CLA	U	8003	-	-	0/0/66/135	0/0/8/9
17	CLA	U	8004	-	-	0/0/66/135	0/0/8/9
17	CLA	U	8005	-	-	0/0/66/135	0/0/8/9
17	CLA	U	8006	-	-	0/0/66/135	0/0/8/9
17	CLA	V	5233	-	-	0/0/66/135	0/0/8/9
17	CLA	V	5701	-	-	0/0/66/135	0/0/8/9
17	CLA	W	5801	-	-	0/0/66/135	0/0/8/9
17	CLA	Z	5101	-	-	0/0/66/135	0/0/8/9
17	CLA	Z	5302	-	-	0/0/66/135	0/0/8/9
17	CLA	Z	8008	-	-	0/0/66/135	0/0/8/9

All (3669) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1023	CLA	C3B-C4B	87.74	1.50	1.38
17	Q	5023	CLA	C3B-C4B	87.40	1.50	1.38
17	B	1232	CLA	C3B-C4B	82.18	1.49	1.38
17	Q	5232	CLA	C3B-C4B	81.88	1.49	1.38
17	P	5128	CLA	C3B-C4B	81.50	1.49	1.38
17	A	1128	CLA	C3B-C4B	81.33	1.49	1.38
17	Q	5212	CLA	C3B-C4B	78.29	1.49	1.38
17	B	1212	CLA	C3B-C4B	77.99	1.49	1.38
17	P	5136	CLA	C3B-C4B	77.73	1.49	1.38
17	A	1136	CLA	C3B-C4B	77.69	1.49	1.38
17	P	5115	CLA	C3B-C4B	77.48	1.49	1.38
17	P	5112	CLA	C3B-C4B	77.46	1.49	1.38
17	A	1115	CLA	C3B-C4B	77.43	1.49	1.38
17	A	1112	CLA	C3B-C4B	77.39	1.49	1.38
17	Q	5022	CLA	C3B-C4B	76.94	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1022	CLA	C3B-C4B	76.90	1.49	1.38
17	P	5118	CLA	C3B-C4B	76.89	1.49	1.38
17	A	1118	CLA	C3B-C4B	76.84	1.49	1.38
17	2	1017	CLA	C3B-C4B	76.66	1.49	1.38
17	0	1016	CLA	C3B-C4B	76.46	1.49	1.38
17	P	5125	CLA	C3B-C4B	76.42	1.49	1.38
17	8	1025	CLA	C3B-C4B	76.40	1.49	1.38
17	U	8005	CLA	C3B-C4B	76.36	1.49	1.38
17	0	1022	CLA	C3B-C4B	76.29	1.49	1.38
17	B	1221	CLA	C3B-C4B	76.25	1.49	1.38
17	4	1015	CLA	C3B-C4B	76.25	1.49	1.38
17	8	1017	CLA	C3B-C4B	76.22	1.49	1.38
17	4	1026	CLA	C3B-C4B	76.19	1.49	1.38
17	Q	5224	CLA	C3B-C4B	76.17	1.49	1.38
17	2	1022	CLA	C3B-C4B	76.17	1.49	1.38
17	A	1125	CLA	C3B-C4B	76.17	1.49	1.38
17	B	1224	CLA	C3B-C4B	76.17	1.49	1.38
17	8	1022	CLA	C3B-C4B	76.13	1.49	1.38
17	1	1023	CLA	C3B-C4B	76.11	1.49	1.38
17	0	1015	CLA	C3B-C4B	76.09	1.49	1.38
17	4	1011	CLA	C3B-C4B	76.06	1.49	1.38
17	5	5404	CLA	C3B-C4B	76.06	1.49	1.38
17	K	1404	CLA	C3B-C4B	76.05	1.49	1.38
17	4	1022	CLA	C3B-C4B	76.04	1.49	1.38
17	Q	5242	CLA	C3B-C4B	76.03	1.49	1.38
17	Q	5221	CLA	C3B-C4B	76.03	1.49	1.38
17	4	1031	CLA	C3B-C4B	76.02	1.49	1.38
17	8	1033	CLA	C3B-C4B	76.02	1.49	1.38
17	7	1011	CLA	C3B-C4B	76.00	1.49	1.38
17	9	1011	CLA	C3B-C4B	75.99	1.49	1.38
17	F	4005	CLA	C3B-C4B	75.98	1.49	1.38
17	4	1016	CLA	C3B-C4B	75.94	1.49	1.38
17	9	1041	CLA	C3B-C4B	75.91	1.49	1.38
17	0	1026	CLA	C3B-C4B	75.89	1.49	1.38
17	1	1011	CLA	C3B-C4B	75.89	1.49	1.38
17	4	1033	CLA	C3B-C4B	75.88	1.49	1.38
17	9	1026	CLA	C3B-C4B	75.88	1.49	1.38
17	P	8010	CLA	C3B-C4B	75.88	1.49	1.38
17	9	1032	CLA	C3B-C4B	75.85	1.49	1.38
17	B	1242	CLA	C3B-C4B	75.84	1.49	1.38
17	7	1017	CLA	C3B-C4B	75.82	1.49	1.38
17	0	1032	CLA	C3B-C4B	75.81	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Z	8008	CLA	C3B-C4B	75.81	1.49	1.38
17	3	1041	CLA	C3B-C4B	75.80	1.49	1.38
17	0	1031	CLA	C3B-C4B	75.79	1.49	1.38
17	4	1032	CLA	C3B-C4B	75.79	1.49	1.38
17	2	1025	CLA	C3B-C4B	75.77	1.49	1.38
17	1	1017	CLA	C3B-C4B	75.76	1.49	1.38
17	3	1021	CLA	C3B-C4B	75.74	1.49	1.38
17	0	1011	CLA	C3B-C4B	75.73	1.49	1.38
17	3	1016	CLA	C3B-C4B	75.72	1.49	1.38
17	3	1026	CLA	C3B-C4B	75.69	1.49	1.38
17	3	1032	CLA	C3B-C4B	75.69	1.49	1.38
17	8	1011	CLA	C3B-C4B	75.67	1.49	1.38
17	F	4004	CLA	C3B-C4B	75.66	1.49	1.38
17	3	1011	CLA	C3B-C4B	75.66	1.49	1.38
17	9	1022	CLA	C3B-C4B	75.65	1.49	1.38
17	B	1241	CLA	C3B-C4B	75.65	1.49	1.38
17	K	1403	CLA	C3B-C4B	75.63	1.49	1.38
17	3	1022	CLA	C3B-C4B	75.63	1.49	1.38
17	9	1016	CLA	C3B-C4B	75.62	1.49	1.38
17	H	1801	CLA	C3B-C4B	75.62	1.49	1.38
17	A	4010	CLA	C3B-C4B	75.60	1.49	1.38
17	5	5403	CLA	C3B-C4B	75.59	1.49	1.38
17	2	1033	CLA	C3B-C4B	75.59	1.49	1.38
17	0	8002	CLA	C3B-C4B	75.59	1.49	1.38
17	7	1013	CLA	C3B-C4B	75.56	1.49	1.38
17	2	1013	CLA	C3B-C4B	75.54	1.49	1.38
17	2	4007	CLA	C3B-C4B	75.54	1.49	1.38
17	7	1016	CLA	C3B-C4B	75.53	1.49	1.38
17	U	8004	CLA	C3B-C4B	75.53	1.49	1.38
17	7	1025	CLA	C3B-C4B	75.51	1.49	1.38
17	4	1012	CLA	C3B-C4B	75.50	1.49	1.38
17	J	4008	CLA	C3B-C4B	75.50	1.49	1.38
17	8	8007	CLA	C3B-C4B	75.50	1.49	1.38
17	3	1015	CLA	C3B-C4B	75.47	1.49	1.38
17	2	1031	CLA	C3B-C4B	75.47	1.49	1.38
17	J	1101	CLA	C3B-C4B	75.47	1.49	1.38
17	W	5801	CLA	C3B-C4B	75.47	1.49	1.38
17	1	1016	CLA	C3B-C4B	75.46	1.49	1.38
17	1	1021	CLA	C3B-C4B	75.45	1.49	1.38
17	1	1013	CLA	C3B-C4B	75.45	1.49	1.38
17	2	1011	CLA	C3B-C4B	75.45	1.49	1.38
17	8	1013	CLA	C3B-C4B	75.44	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	0	1033	CLA	C3B-C4B	75.44	1.49	1.38
17	1	1022	CLA	C3B-C4B	75.44	1.49	1.38
17	6	5504	CLA	C3B-C4B	75.44	1.49	1.38
17	0	1012	CLA	C3B-C4B	75.44	1.49	1.38
17	Z	5101	CLA	C3B-C4B	75.43	1.49	1.38
17	7	1023	CLA	C3B-C4B	75.43	1.49	1.38
17	0	1025	CLA	C3B-C4B	75.43	1.49	1.38
17	Q	5241	CLA	C3B-C4B	75.42	1.49	1.38
17	8	1023	CLA	C3B-C4B	75.42	1.49	1.38
17	9	1033	CLA	C3B-C4B	75.40	1.49	1.38
17	7	1022	CLA	C3B-C4B	75.39	1.49	1.38
17	9	1015	CLA	C3B-C4B	75.39	1.49	1.38
17	1	1012	CLA	C3B-C4B	75.38	1.49	1.38
17	8	1015	CLA	C3B-C4B	75.38	1.49	1.38
17	7	1021	CLA	C3B-C4B	75.37	1.49	1.38
17	8	1031	CLA	C3B-C4B	75.36	1.49	1.38
17	B	1235	CLA	C3B-C4B	75.35	1.49	1.38
17	V	5701	CLA	C3B-C4B	75.35	1.49	1.38
17	9	1021	CLA	C3B-C4B	75.35	1.49	1.38
17	8	1016	CLA	C3B-C4B	75.34	1.49	1.38
17	2	1015	CLA	C3B-C4B	75.33	1.49	1.38
17	G	1701	CLA	C3B-C4B	75.33	1.49	1.38
17	1	1025	CLA	C3B-C4B	75.33	1.49	1.38
17	0	1014	CLA	C3B-C4B	75.33	1.49	1.38
17	4	1013	CLA	C3B-C4B	75.29	1.49	1.38
17	2	1023	CLA	C3B-C4B	75.27	1.49	1.38
17	Q	5240	CLA	C3B-C4B	75.27	1.49	1.38
17	4	1021	CLA	C3B-C4B	75.27	1.49	1.38
17	8	1021	CLA	C3B-C4B	75.26	1.49	1.38
17	4	1025	CLA	C3B-C4B	75.26	1.49	1.38
17	3	1033	CLA	C3B-C4B	75.25	1.48	1.38
17	7	1012	CLA	C3B-C4B	75.24	1.48	1.38
17	F	4006	CLA	C3B-C4B	75.23	1.48	1.38
17	9	1017	CLA	C3B-C4B	75.23	1.48	1.38
17	7	1031	CLA	C3B-C4B	75.23	1.48	1.38
17	2	1012	CLA	C3B-C4B	75.23	1.48	1.38
17	B	1240	CLA	C3B-C4B	75.23	1.48	1.38
17	1	1015	CLA	C3B-C4B	75.21	1.48	1.38
17	P	8009	CLA	C3B-C4B	75.21	1.48	1.38
17	0	1021	CLA	C3B-C4B	75.20	1.48	1.38
17	3	1017	CLA	C3B-C4B	75.20	1.48	1.38
17	8	1012	CLA	C3B-C4B	75.19	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	1031	CLA	C3B-C4B	75.18	1.48	1.38
17	4	1023	CLA	C3B-C4B	75.17	1.48	1.38
17	4	4002	CLA	C3B-C4B	75.14	1.48	1.38
17	4	1014	CLA	C3B-C4B	75.13	1.48	1.38
17	0	1013	CLA	C3B-C4B	75.12	1.48	1.38
17	A	4009	CLA	C3B-C4B	75.12	1.48	1.38
17	3	1012	CLA	C3B-C4B	75.10	1.48	1.38
17	U	8006	CLA	C3B-C4B	75.10	1.48	1.38
17	3	1014	CLA	C3B-C4B	75.10	1.48	1.38
17	B	4001	CLA	C3B-C4B	75.10	1.48	1.38
17	2	1016	CLA	C3B-C4B	75.06	1.48	1.38
17	L	1504	CLA	C3B-C4B	75.04	1.48	1.38
17	7	1015	CLA	C3B-C4B	75.04	1.48	1.38
17	3	1031	CLA	C3B-C4B	75.02	1.48	1.38
17	2	1026	CLA	C3B-C4B	74.98	1.48	1.38
17	2	1021	CLA	C3B-C4B	74.97	1.48	1.38
17	8	1014	CLA	C3B-C4B	74.97	1.48	1.38
17	0	1017	CLA	C3B-C4B	74.95	1.48	1.38
17	1	1014	CLA	C3B-C4B	74.90	1.48	1.38
17	2	1014	CLA	C3B-C4B	74.85	1.48	1.38
17	9	1014	CLA	C3B-C4B	74.84	1.48	1.38
17	7	1014	CLA	C3B-C4B	74.84	1.48	1.38
17	8	1026	CLA	C3B-C4B	74.78	1.48	1.38
17	Q	5235	CLA	C3B-C4B	74.76	1.48	1.38
17	1	1031	CLA	C3B-C4B	74.75	1.48	1.38
17	B	1219	CLA	C3B-C4B	74.75	1.48	1.38
17	Q	5219	CLA	C3B-C4B	74.72	1.48	1.38
17	Q	5218	CLA	C3B-C4B	74.72	1.48	1.38
17	3	1025	CLA	C3B-C4B	74.71	1.48	1.38
17	0	1023	CLA	C3B-C4B	74.68	1.48	1.38
17	Q	8001	CLA	C3B-C4B	74.61	1.48	1.38
17	B	1218	CLA	C3B-C4B	74.61	1.48	1.38
17	9	1012	CLA	C3B-C4B	74.54	1.48	1.38
17	4	1017	CLA	C3B-C4B	74.52	1.48	1.38
17	Q	5228	CLA	C3B-C4B	74.49	1.48	1.38
17	A	1140	CLA	C3B-C4B	74.33	1.48	1.38
17	1	1026	CLA	C3B-C4B	74.32	1.48	1.38
17	7	1026	CLA	C3B-C4B	74.28	1.48	1.38
17	B	1228	CLA	C3B-C4B	74.14	1.48	1.38
17	9	1025	CLA	C3B-C4B	74.11	1.48	1.38
17	F	4003	CLA	C3B-C4B	74.06	1.48	1.38
17	U	5229	CLA	C3B-C4B	74.01	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5213	CLA	C3B-C4B	73.96	1.48	1.38
17	P	5140	CLA	C3B-C4B	73.92	1.48	1.38
17	Q	5220	CLA	C3B-C4B	73.82	1.48	1.38
17	P	5901	CLA	C3B-C4B	73.72	1.48	1.38
17	U	8003	CLA	C3B-C4B	73.71	1.48	1.38
17	P	5129	CLA	C3B-C4B	73.69	1.48	1.38
17	F	1301	CLA	C3B-C4B	73.68	1.48	1.38
17	Q	5214	CLA	C3B-C4B	73.68	1.48	1.38
17	F	1229	CLA	C3B-C4B	73.67	1.48	1.38
17	A	1901	CLA	C3B-C4B	73.58	1.48	1.38
17	B	1213	CLA	C3B-C4B	73.52	1.48	1.38
17	B	1214	CLA	C3B-C4B	73.52	1.48	1.38
17	B	1220	CLA	C3B-C4B	73.46	1.48	1.38
17	Q	5204	CLA	C3B-C4B	73.32	1.48	1.38
17	B	1204	CLA	C3B-C4B	73.31	1.48	1.38
17	B	1234	CLA	C3B-C4B	73.21	1.48	1.38
17	P	5123	CLA	C3B-C4B	73.20	1.48	1.38
17	A	1123	CLA	C3B-C4B	73.17	1.48	1.38
17	U	5301	CLA	C3B-C4B	73.14	1.48	1.38
17	A	1129	CLA	C3B-C4B	73.03	1.48	1.38
17	Q	5234	CLA	C3B-C4B	72.98	1.48	1.38
17	6	5501	CLA	C3B-C4B	72.85	1.48	1.38
17	P	5119	CLA	C3B-C4B	72.84	1.48	1.38
17	L	1501	CLA	C3B-C4B	72.81	1.48	1.38
17	A	1119	CLA	C3B-C4B	72.65	1.48	1.38
17	B	1231	CLA	C3B-C4B	72.57	1.48	1.38
17	P	5138	CLA	C3B-C4B	72.51	1.48	1.38
17	Q	5231	CLA	C3B-C4B	72.50	1.48	1.38
17	A	1138	CLA	C3B-C4B	72.28	1.48	1.38
17	A	1120	CLA	C3B-C4B	72.24	1.48	1.38
17	P	5120	CLA	C3B-C4B	72.02	1.48	1.38
17	B	1209	CLA	C3B-C4B	71.93	1.48	1.38
17	Q	5209	CLA	C3B-C4B	71.88	1.48	1.38
17	P	5134	CLA	C3B-C4B	71.14	1.48	1.38
17	A	1116	CLA	C3B-C4B	71.03	1.48	1.38
17	A	1134	CLA	C3B-C4B	71.00	1.48	1.38
17	P	5116	CLA	C3B-C4B	70.92	1.48	1.38
17	Q	5223	CLA	C3B-C4B	70.85	1.48	1.38
17	G	1233	CLA	C3B-C4B	70.84	1.48	1.38
17	A	1106	CLA	C3B-C4B	70.80	1.48	1.38
17	V	5233	CLA	C3B-C4B	70.79	1.48	1.38
17	B	1223	CLA	C3B-C4B	70.77	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5106	CLA	C3B-C4B	70.75	1.48	1.38
17	A	1110	CLA	C3B-C4B	70.71	1.48	1.38
17	A	1121	CLA	C3B-C4B	70.62	1.48	1.38
17	B	1207	CLA	C2B-C1B	70.60	1.48	1.38
17	Q	5207	CLA	C2B-C1B	70.54	1.48	1.38
17	Q	5130	CLA	C2B-C1B	70.50	1.48	1.38
17	P	5121	CLA	C3B-C4B	70.45	1.48	1.38
17	B	1130	CLA	C2B-C1B	70.37	1.48	1.38
17	K	1401	CLA	C3B-C4B	70.36	1.48	1.38
17	6	5502	CLA	C3B-C4B	70.33	1.48	1.38
17	L	1502	CLA	C3B-C4B	70.20	1.48	1.38
17	5	5401	CLA	C3B-C4B	70.17	1.48	1.38
17	P	5110	CLA	C3B-C4B	70.15	1.48	1.38
17	P	5135	CLA	C2B-C1B	69.85	1.48	1.38
17	A	1135	CLA	C2B-C1B	69.76	1.48	1.38
17	P	5402	CLA	C3B-C4B	69.73	1.48	1.38
17	A	1402	CLA	C3B-C4B	69.21	1.48	1.38
17	6	5503	CLA	C3B-C4B	69.01	1.48	1.38
17	B	1201	CLA	C3B-C4B	68.96	1.48	1.38
17	P	5104	CLA	C3B-C4B	68.96	1.48	1.38
17	J	1302	CLA	C3B-C4B	68.81	1.48	1.38
17	Z	5302	CLA	C3B-C4B	68.79	1.48	1.38
17	Q	5217	CLA	C3B-C4B	68.69	1.48	1.38
17	Q	5201	CLA	C3B-C4B	68.67	1.48	1.38
17	Q	5216	CLA	C3B-C4B	68.65	1.48	1.38
17	B	1216	CLA	C3B-C4B	68.58	1.48	1.38
17	L	1503	CLA	C3B-C4B	68.52	1.48	1.38
17	B	1217	CLA	C3B-C4B	68.50	1.48	1.38
17	A	1104	CLA	C3B-C4B	68.36	1.48	1.38
17	P	5013	CLA	C3B-C4B	68.36	1.48	1.38
17	B	1205	CLA	C3B-C4B	68.35	1.48	1.38
17	Q	5205	CLA	C3B-C4B	68.18	1.48	1.38
17	P	5105	CLA	C3B-C4B	67.77	1.47	1.38
17	P	5109	CLA	C3B-C4B	67.74	1.47	1.38
17	A	1013	CLA	C3B-C4B	67.74	1.47	1.38
17	P	5114	CLA	C3B-C4B	67.70	1.47	1.38
17	A	1109	CLA	C3B-C4B	67.62	1.47	1.38
17	A	1114	CLA	C3B-C4B	67.57	1.47	1.38
17	A	1105	CLA	C3B-C4B	67.34	1.47	1.38
17	B	1208	CLA	C3B-C4B	67.19	1.47	1.38
17	Q	5208	CLA	C3B-C4B	67.11	1.47	1.38
17	B	1210	CLA	C3B-C4B	66.81	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5210	CLA	C3B-C4B	66.73	1.47	1.38
17	Q	5227	CLA	C3B-C4B	66.68	1.47	1.38
17	P	5011	CLA	C2B-C1B	66.35	1.47	1.38
17	Q	5130	CLA	C3B-C4B	66.33	1.47	1.38
17	B	1227	CLA	C3B-C4B	66.08	1.47	1.38
17	B	1130	CLA	C3B-C4B	65.93	1.47	1.38
17	A	1126	CLA	C3B-C4B	65.64	1.47	1.38
17	B	1230	CLA	C3B-C4B	65.59	1.47	1.38
17	Q	5207	CLA	C3B-C4B	65.52	1.47	1.38
17	A	1011	CLA	C2B-C1B	65.50	1.47	1.38
17	P	5126	CLA	C3B-C4B	65.48	1.47	1.38
17	B	1231	CLA	C2B-C1B	65.43	1.47	1.38
17	Q	5230	CLA	C3B-C4B	65.24	1.47	1.38
17	B	1207	CLA	C3B-C4B	65.21	1.47	1.38
17	P	5111	CLA	C3B-C4B	65.20	1.47	1.38
17	A	1111	CLA	C3B-C4B	65.08	1.47	1.38
17	Q	5203	CLA	C2B-C1B	64.95	1.47	1.38
17	Q	5231	CLA	C2B-C1B	64.76	1.47	1.38
17	Q	5203	CLA	C3B-C4B	64.46	1.47	1.38
17	B	1203	CLA	C2B-C1B	64.38	1.47	1.38
17	B	1237	CLA	C3B-C4B	64.33	1.47	1.38
17	Q	5237	CLA	C3B-C4B	64.23	1.47	1.38
17	F	1301	CLA	C2B-C1B	64.23	1.47	1.38
17	U	5301	CLA	C2B-C1B	63.96	1.47	1.38
17	B	1203	CLA	C3B-C4B	63.67	1.47	1.38
17	P	5012	CLA	C3B-C4B	63.61	1.47	1.38
17	P	5137	CLA	C3B-C4B	63.56	1.47	1.38
17	A	1137	CLA	C3B-C4B	63.48	1.47	1.38
17	A	1012	CLA	C3B-C4B	63.44	1.47	1.38
17	P	5107	CLA	C3B-C4B	63.36	1.47	1.38
17	P	5111	CLA	C2B-C1B	63.07	1.47	1.38
17	A	1402	CLA	C2B-C1B	63.06	1.47	1.38
17	P	5402	CLA	C2B-C1B	62.98	1.47	1.38
17	A	1107	CLA	C3B-C4B	62.78	1.47	1.38
17	A	1124	CLA	C3B-C4B	62.63	1.47	1.38
17	Q	5225	CLA	C3B-C4B	62.59	1.47	1.38
17	A	1111	CLA	C2B-C1B	62.58	1.47	1.38
17	B	1223	CLA	C2B-C1B	62.54	1.47	1.38
17	B	1225	CLA	C3B-C4B	62.53	1.47	1.38
17	Q	5223	CLA	C2B-C1B	62.48	1.47	1.38
17	P	5108	CLA	C3B-C4B	62.41	1.47	1.38
17	P	5124	CLA	C3B-C4B	62.32	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1211	CLA	C3B-C4B	62.25	1.47	1.38
17	B	1205	CLA	C2B-C1B	62.24	1.47	1.38
17	A	1102	CLA	C3B-C4B	62.24	1.47	1.38
17	P	5102	CLA	C3B-C4B	62.22	1.47	1.38
17	Q	5222	CLA	C3B-C4B	62.21	1.47	1.38
17	P	5113	CLA	C3B-C4B	62.11	1.47	1.38
17	A	1108	CLA	C3B-C4B	62.06	1.47	1.38
17	B	1021	CLA	C3B-C4B	62.04	1.47	1.38
17	Q	5021	CLA	C3B-C4B	62.00	1.47	1.38
17	P	5133	CLA	C3B-C4B	62.00	1.47	1.38
17	P	5125	CLA	C2B-C1B	61.96	1.47	1.38
17	A	1113	CLA	C3B-C4B	61.96	1.47	1.38
17	A	1133	CLA	C3B-C4B	61.96	1.47	1.38
17	P	5136	CLA	C2B-C1B	61.92	1.47	1.38
17	Q	5205	CLA	C2B-C1B	61.88	1.47	1.38
17	Q	5211	CLA	C3B-C4B	61.85	1.47	1.38
17	B	1222	CLA	C3B-C4B	61.84	1.47	1.38
17	P	5137	CLA	C2B-C1B	61.83	1.47	1.38
17	A	1125	CLA	C2B-C1B	61.72	1.47	1.38
17	B	1219	CLA	C2B-C1B	61.63	1.47	1.38
17	A	1136	CLA	C2B-C1B	61.54	1.47	1.38
17	A	1137	CLA	C2B-C1B	61.29	1.47	1.38
17	A	1118	CLA	C2B-C1B	61.08	1.47	1.38
17	Q	5219	CLA	C2B-C1B	61.06	1.47	1.38
17	B	1236	CLA	C3B-C4B	60.93	1.47	1.38
17	P	5118	CLA	C2B-C1B	60.58	1.47	1.38
17	Q	5236	CLA	C3B-C4B	60.43	1.47	1.38
17	V	5233	CLA	C2B-C1B	60.12	1.46	1.38
17	B	1209	CLA	C2B-C1B	60.07	1.46	1.38
17	L	1502	CLA	C2B-C1B	60.04	1.46	1.38
17	Q	5202	CLA	C2B-C1B	59.96	1.46	1.38
17	G	1233	CLA	C2B-C1B	59.88	1.46	1.38
17	B	1202	CLA	C2B-C1B	59.80	1.46	1.38
17	6	5502	CLA	C2B-C1B	59.77	1.46	1.38
17	6	5501	CLA	C2B-C1B	59.74	1.46	1.38
17	A	1109	CLA	C2B-C1B	59.64	1.46	1.38
17	Q	5209	CLA	C2B-C1B	59.58	1.46	1.38
17	B	1204	CLA	C2B-C1B	59.51	1.46	1.38
17	P	5134	CLA	C2B-C1B	59.47	1.46	1.38
17	A	1134	CLA	C2B-C1B	59.41	1.46	1.38
17	P	5109	CLA	C2B-C1B	59.34	1.46	1.38
17	Q	5210	CLA	C2B-C1B	59.29	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1105	CLA	C2B-C1B	59.26	1.46	1.38
17	Q	5204	CLA	C2B-C1B	59.23	1.46	1.38
17	B	1210	CLA	C2B-C1B	59.14	1.46	1.38
17	L	1501	CLA	C2B-C1B	59.11	1.46	1.38
17	P	5110	CLA	C2B-C1B	59.06	1.46	1.38
17	P	5105	CLA	C2B-C1B	59.05	1.46	1.38
17	A	1110	CLA	C2B-C1B	58.91	1.46	1.38
17	P	5013	CLA	C2B-C1B	58.74	1.46	1.38
17	A	1013	CLA	C2B-C1B	58.73	1.46	1.38
17	A	1104	CLA	C2B-C1B	58.60	1.46	1.38
17	A	1138	CLA	C2B-C1B	58.41	1.46	1.38
17	P	5138	CLA	C2B-C1B	58.30	1.46	1.38
17	P	5104	CLA	C2B-C1B	58.22	1.46	1.38
17	Q	5217	CLA	C2B-C1B	58.20	1.46	1.38
17	Q	5226	CLA	C2B-C1B	58.15	1.46	1.38
17	B	1217	CLA	C2B-C1B	58.11	1.46	1.38
17	P	5122	CLA	C3B-C4B	58.10	1.46	1.38
17	P	5117	CLA	C3B-C4B	58.05	1.46	1.38
17	Q	5238	CLA	C2B-C1B	58.02	1.46	1.38
17	A	1117	CLA	C3B-C4B	58.01	1.46	1.38
17	P	5112	CLA	C2B-C1B	57.96	1.46	1.38
17	P	5113	CLA	C2B-C1B	57.93	1.46	1.38
17	B	1230	CLA	C2B-C1B	57.85	1.46	1.38
17	A	1122	CLA	C3B-C4B	57.82	1.46	1.38
17	Q	5230	CLA	C2B-C1B	57.78	1.46	1.38
17	B	1238	CLA	C2B-C1B	57.71	1.46	1.38
17	B	1226	CLA	C2B-C1B	57.58	1.46	1.38
17	B	1222	CLA	C2B-C1B	57.48	1.46	1.38
17	Q	5222	CLA	C2B-C1B	57.47	1.46	1.38
17	A	1112	CLA	C2B-C1B	57.43	1.46	1.38
17	P	5103	CLA	C3B-C4B	57.39	1.46	1.38
17	K	1401	CLA	C2B-C1B	57.34	1.46	1.38
17	5	5401	CLA	C2B-C1B	57.26	1.46	1.38
17	A	1113	CLA	C2B-C1B	57.24	1.46	1.38
17	P	5131	CLA	C2B-C1B	57.13	1.46	1.38
17	B	1218	CLA	C2B-C1B	57.09	1.46	1.38
17	A	1131	CLA	C2B-C1B	57.05	1.46	1.38
17	A	1103	CLA	C3B-C4B	56.99	1.46	1.38
17	P	5126	CLA	C2B-C1B	56.99	1.46	1.38
17	Q	5218	CLA	C2B-C1B	56.96	1.46	1.38
17	Q	5023	CLA	C2B-C1B	56.89	1.46	1.38
17	B	1234	CLA	C2B-C1B	56.87	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1126	CLA	C2B-C1B	56.84	1.46	1.38
17	B	1023	CLA	C2B-C1B	56.83	1.46	1.38
17	Q	5234	CLA	C2B-C1B	56.82	1.46	1.38
17	Q	5202	CLA	C3B-C4B	56.78	1.46	1.38
17	P	5128	CLA	C2B-C1B	56.69	1.46	1.38
17	B	1226	CLA	C3B-C4B	56.61	1.46	1.38
17	A	1128	CLA	C2B-C1B	56.41	1.46	1.38
17	A	1139	CLA	C3B-C4B	56.32	1.46	1.38
17	A	1115	CLA	C2B-C1B	56.32	1.46	1.38
17	Q	5226	CLA	C3B-C4B	56.27	1.46	1.38
17	P	5115	CLA	C2B-C1B	56.26	1.46	1.38
17	B	1202	CLA	C3B-C4B	56.24	1.46	1.38
17	P	5139	CLA	C3B-C4B	56.22	1.46	1.38
17	Q	5021	CLA	C2B-C1B	55.89	1.46	1.38
17	B	1215	CLA	C3B-C4B	55.80	1.46	1.38
17	A	1123	CLA	C2B-C1B	55.63	1.46	1.38
17	Q	5215	CLA	C3B-C4B	55.62	1.46	1.38
17	P	5123	CLA	C2B-C1B	55.46	1.46	1.38
17	A	1139	CLA	C2B-C1B	55.40	1.46	1.38
17	B	1021	CLA	C2B-C1B	55.34	1.46	1.38
17	4	1012	CLA	C2B-C1B	55.32	1.46	1.38
17	P	5139	CLA	C2B-C1B	55.14	1.46	1.38
17	P	5140	CLA	C2B-C1B	55.13	1.46	1.38
17	P	5135	CLA	C3B-C4B	55.04	1.46	1.38
17	A	1103	CLA	C2B-C1B	55.02	1.46	1.38
17	A	1140	CLA	C2B-C1B	54.90	1.46	1.38
17	Q	5220	CLA	C2B-C1B	54.88	1.46	1.38
17	B	1220	CLA	C2B-C1B	54.76	1.46	1.38
17	P	5103	CLA	C2B-C1B	54.72	1.46	1.38
17	A	1135	CLA	C3B-C4B	54.65	1.46	1.38
17	P	5121	CLA	C2B-C1B	54.65	1.46	1.38
17	B	1215	CLA	C2B-C1B	54.58	1.46	1.38
17	0	1012	CLA	C2B-C1B	54.53	1.46	1.38
17	A	1121	CLA	C2B-C1B	54.50	1.46	1.38
17	V	5701	CLA	C2B-C1B	54.43	1.46	1.38
17	A	1127	CLA	C2B-C1B	54.42	1.46	1.38
17	0	1022	CLA	C2B-C1B	54.39	1.46	1.38
17	0	1021	CLA	C2B-C1B	54.36	1.46	1.38
17	B	1208	CLA	C2B-C1B	54.36	1.46	1.38
17	3	1032	CLA	C2B-C1B	54.33	1.46	1.38
17	0	1015	CLA	C2B-C1B	54.31	1.46	1.38
17	P	5127	CLA	C2B-C1B	54.31	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	5403	CLA	C2B-C1B	54.31	1.46	1.38
17	A	1116	CLA	C2B-C1B	54.30	1.46	1.38
17	1	1014	CLA	C2B-C1B	54.30	1.46	1.38
17	4	4002	CLA	C2B-C1B	54.22	1.46	1.38
17	8	1017	CLA	C2B-C1B	54.21	1.46	1.38
17	9	1032	CLA	C2B-C1B	54.21	1.46	1.38
17	Q	5215	CLA	C2B-C1B	54.19	1.46	1.38
17	8	1026	CLA	C2B-C1B	54.18	1.46	1.38
17	2	1017	CLA	C2B-C1B	54.16	1.46	1.38
17	W	5801	CLA	C2B-C1B	54.16	1.46	1.38
17	9	1014	CLA	C2B-C1B	54.13	1.46	1.38
17	9	1033	CLA	C2B-C1B	54.10	1.46	1.38
17	Q	5235	CLA	C2B-C1B	54.09	1.46	1.38
17	0	1013	CLA	C2B-C1B	54.07	1.46	1.38
17	4	1013	CLA	C2B-C1B	54.05	1.46	1.38
17	2	4007	CLA	C2B-C1B	54.02	1.46	1.38
17	Q	8001	CLA	C2B-C1B	54.01	1.46	1.38
17	3	1014	CLA	C2B-C1B	54.01	1.46	1.38
17	5	5404	CLA	C2B-C1B	54.01	1.46	1.38
17	1	1023	CLA	C2B-C1B	54.00	1.46	1.38
17	P	5116	CLA	C2B-C1B	54.00	1.46	1.38
17	G	1701	CLA	C2B-C1B	53.98	1.46	1.38
17	B	1213	CLA	C2B-C1B	53.98	1.46	1.38
17	Q	5241	CLA	C2B-C1B	53.98	1.46	1.38
17	B	4001	CLA	C2B-C1B	53.98	1.46	1.38
17	7	1017	CLA	C2B-C1B	53.97	1.46	1.38
17	F	4006	CLA	C2B-C1B	53.97	1.46	1.38
17	K	1403	CLA	C2B-C1B	53.97	1.46	1.38
17	4	1022	CLA	C2B-C1B	53.97	1.46	1.38
17	4	1033	CLA	C2B-C1B	53.97	1.46	1.38
17	4	1021	CLA	C2B-C1B	53.95	1.46	1.38
17	1	1011	CLA	C2B-C1B	53.93	1.46	1.38
17	4	1015	CLA	C2B-C1B	53.92	1.46	1.38
17	7	1012	CLA	C2B-C1B	53.90	1.46	1.38
17	8	8007	CLA	C2B-C1B	53.90	1.46	1.38
17	K	1404	CLA	C2B-C1B	53.90	1.46	1.38
17	0	8002	CLA	C2B-C1B	53.87	1.46	1.38
17	B	1221	CLA	C2B-C1B	53.87	1.46	1.38
17	Q	5213	CLA	C2B-C1B	53.85	1.46	1.38
17	3	1017	CLA	C2B-C1B	53.85	1.46	1.38
17	7	1014	CLA	C2B-C1B	53.84	1.46	1.38
17	2	1026	CLA	C2B-C1B	53.83	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1241	CLA	C2B-C1B	53.81	1.46	1.38
17	Q	5228	CLA	C2B-C1B	53.81	1.46	1.38
17	H	1801	CLA	C2B-C1B	53.81	1.46	1.38
17	B	1235	CLA	C2B-C1B	53.79	1.46	1.38
17	0	1033	CLA	C2B-C1B	53.79	1.46	1.38
17	7	1023	CLA	C2B-C1B	53.72	1.46	1.38
17	3	1012	CLA	C2B-C1B	53.70	1.46	1.38
17	2	1011	CLA	C2B-C1B	53.70	1.46	1.38
17	8	1011	CLA	C2B-C1B	53.67	1.46	1.38
17	8	1033	CLA	C2B-C1B	53.67	1.46	1.38
17	1	1031	CLA	C2B-C1B	53.65	1.46	1.38
17	9	1031	CLA	C2B-C1B	53.64	1.46	1.38
17	4	1011	CLA	C2B-C1B	53.64	1.46	1.38
17	1	1017	CLA	C2B-C1B	53.64	1.46	1.38
17	7	1031	CLA	C2B-C1B	53.63	1.46	1.38
17	8	1022	CLA	C2B-C1B	53.63	1.46	1.38
17	Q	5208	CLA	C2B-C1B	53.62	1.46	1.38
17	Z	8008	CLA	C2B-C1B	53.61	1.46	1.38
17	B	1242	CLA	C2B-C1B	53.60	1.46	1.38
17	9	1017	CLA	C2B-C1B	53.58	1.46	1.38
17	L	1504	CLA	C2B-C1B	53.56	1.46	1.38
17	3	1033	CLA	C2B-C1B	53.55	1.46	1.38
17	Q	5221	CLA	C2B-C1B	53.55	1.46	1.38
17	2	1033	CLA	C2B-C1B	53.53	1.46	1.38
17	J	1101	CLA	C2B-C1B	53.52	1.46	1.38
17	4	1017	CLA	C2B-C1B	53.52	1.46	1.38
17	7	1011	CLA	C2B-C1B	53.51	1.46	1.38
17	2	1022	CLA	C2B-C1B	53.51	1.46	1.38
17	3	1031	CLA	C2B-C1B	53.48	1.46	1.38
17	0	1011	CLA	C2B-C1B	53.48	1.46	1.38
17	P	5133	CLA	C2B-C1B	53.48	1.46	1.38
17	0	1017	CLA	C2B-C1B	53.47	1.46	1.38
17	1	1025	CLA	C2B-C1B	53.47	1.46	1.38
17	4	1014	CLA	C2B-C1B	53.46	1.46	1.38
17	8	1021	CLA	C2B-C1B	53.46	1.46	1.38
17	8	1023	CLA	C2B-C1B	53.45	1.46	1.38
17	3	1011	CLA	C2B-C1B	53.44	1.46	1.38
17	U	8004	CLA	C2B-C1B	53.44	1.46	1.38
17	J	4008	CLA	C2B-C1B	53.44	1.46	1.38
17	A	4010	CLA	C2B-C1B	53.43	1.46	1.38
17	A	4009	CLA	C2B-C1B	53.43	1.46	1.38
17	2	1013	CLA	C2B-C1B	53.42	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	4003	CLA	C2B-C1B	53.41	1.46	1.38
17	9	1012	CLA	C2B-C1B	53.40	1.46	1.38
17	8	1013	CLA	C2B-C1B	53.38	1.46	1.38
17	8	1016	CLA	C2B-C1B	53.38	1.46	1.38
17	1	1013	CLA	C2B-C1B	53.38	1.46	1.38
17	4	1026	CLA	C2B-C1B	53.38	1.46	1.38
17	7	1025	CLA	C2B-C1B	53.38	1.46	1.38
17	7	1026	CLA	C2B-C1B	53.36	1.46	1.38
17	Z	5101	CLA	C2B-C1B	53.35	1.46	1.38
17	9	1011	CLA	C2B-C1B	53.35	1.46	1.38
17	9	1026	CLA	C2B-C1B	53.34	1.46	1.38
17	2	1012	CLA	C2B-C1B	53.34	1.46	1.38
17	9	1025	CLA	C2B-C1B	53.33	1.46	1.38
17	1	1026	CLA	C2B-C1B	53.33	1.46	1.38
17	2	1023	CLA	C2B-C1B	53.32	1.46	1.38
17	1	1016	CLA	C2B-C1B	53.32	1.46	1.38
17	Q	5242	CLA	C2B-C1B	53.32	1.46	1.38
17	U	8006	CLA	C2B-C1B	53.31	1.46	1.38
17	Q	5239	CLA	C2B-C1B	53.29	1.46	1.38
17	2	1016	CLA	C2B-C1B	53.29	1.46	1.38
17	0	1031	CLA	C2B-C1B	53.29	1.46	1.38
17	2	1021	CLA	C2B-C1B	53.29	1.46	1.38
17	0	1032	CLA	C2B-C1B	53.29	1.46	1.38
17	0	1026	CLA	C2B-C1B	53.27	1.46	1.38
17	4	1032	CLA	C2B-C1B	53.27	1.46	1.38
17	4	1025	CLA	C2B-C1B	53.27	1.46	1.38
17	2	1031	CLA	C2B-C1B	53.27	1.46	1.38
17	9	1015	CLA	C2B-C1B	53.26	1.46	1.38
17	0	1016	CLA	C2B-C1B	53.26	1.46	1.38
17	2	1025	CLA	C2B-C1B	53.26	1.46	1.38
17	J	1302	CLA	C2B-C1B	53.26	1.46	1.38
17	F	4004	CLA	C2B-C1B	53.25	1.46	1.38
17	9	1021	CLA	C2B-C1B	53.25	1.46	1.38
17	6	5504	CLA	C2B-C1B	53.25	1.46	1.38
17	3	1021	CLA	C2B-C1B	53.23	1.46	1.38
17	Z	5302	CLA	C2B-C1B	53.23	1.46	1.38
17	4	1031	CLA	C2B-C1B	53.22	1.46	1.38
17	7	1015	CLA	C2B-C1B	53.22	1.46	1.38
17	3	1015	CLA	C2B-C1B	53.21	1.46	1.38
17	7	1013	CLA	C2B-C1B	53.21	1.46	1.38
17	3	1041	CLA	C2B-C1B	53.20	1.46	1.38
17	9	1041	CLA	C2B-C1B	53.18	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	1012	CLA	C2B-C1B	53.18	1.46	1.38
17	0	1014	CLA	C2B-C1B	53.18	1.46	1.38
17	4	1016	CLA	C2B-C1B	53.18	1.46	1.38
17	1	1015	CLA	C2B-C1B	53.17	1.46	1.38
17	B	1240	CLA	C2B-C1B	53.17	1.46	1.38
17	8	1025	CLA	C2B-C1B	53.16	1.46	1.38
17	A	1133	CLA	C2B-C1B	53.12	1.46	1.38
17	8	1031	CLA	C2B-C1B	53.10	1.46	1.38
17	0	1025	CLA	C2B-C1B	53.08	1.46	1.38
17	B	1239	CLA	C2B-C1B	53.06	1.46	1.38
17	8	1012	CLA	C2B-C1B	53.06	1.46	1.38
17	B	1228	CLA	C2B-C1B	53.06	1.46	1.38
17	P	5127	CLA	C3B-C4B	53.06	1.46	1.38
17	8	1015	CLA	C2B-C1B	53.03	1.46	1.38
17	B	1236	CLA	C2B-C1B	53.01	1.46	1.38
17	3	1026	CLA	C2B-C1B	53.00	1.46	1.38
17	1	1021	CLA	C2B-C1B	52.97	1.45	1.38
17	3	1025	CLA	C2B-C1B	52.96	1.45	1.38
17	7	1022	CLA	C2B-C1B	52.94	1.45	1.38
17	B	1201	CLA	C2B-C1B	52.93	1.45	1.38
17	U	8003	CLA	C2B-C1B	52.93	1.45	1.38
17	4	1023	CLA	C2B-C1B	52.92	1.45	1.38
17	U	8005	CLA	C2B-C1B	52.86	1.45	1.38
17	A	1127	CLA	C3B-C4B	52.85	1.45	1.38
17	2	1015	CLA	C2B-C1B	52.85	1.45	1.38
17	P	8009	CLA	C2B-C1B	52.80	1.45	1.38
17	P	8010	CLA	C2B-C1B	52.77	1.45	1.38
17	Q	5240	CLA	C2B-C1B	52.76	1.45	1.38
17	7	1016	CLA	C2B-C1B	52.74	1.45	1.38
17	Q	5236	CLA	C2B-C1B	52.74	1.45	1.38
17	2	1014	CLA	C2B-C1B	52.72	1.45	1.38
17	3	1022	CLA	C2B-C1B	52.72	1.45	1.38
17	7	1021	CLA	C2B-C1B	52.71	1.45	1.38
17	0	1023	CLA	C2B-C1B	52.70	1.45	1.38
17	3	1016	CLA	C2B-C1B	52.63	1.45	1.38
17	8	1014	CLA	C2B-C1B	52.60	1.45	1.38
17	9	1016	CLA	C2B-C1B	52.60	1.45	1.38
17	Q	5201	CLA	C2B-C1B	52.57	1.45	1.38
17	P	5114	CLA	C2B-C1B	52.56	1.45	1.38
17	1	1022	CLA	C2B-C1B	52.53	1.45	1.38
17	A	1132	CLA	C2B-C1B	52.51	1.45	1.38
17	9	1022	CLA	C2B-C1B	52.50	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	4005	CLA	C2B-C1B	52.45	1.45	1.38
17	A	1114	CLA	C2B-C1B	52.27	1.45	1.38
17	P	5132	CLA	C2B-C1B	51.95	1.45	1.38
17	Q	5227	CLA	C2B-C1B	51.91	1.45	1.38
17	A	1106	CLA	C2B-C1B	51.84	1.45	1.38
17	B	1227	CLA	C2B-C1B	51.82	1.45	1.38
17	P	5106	CLA	C2B-C1B	51.73	1.45	1.38
17	P	5901	CLA	C2B-C1B	51.41	1.45	1.38
17	P	5012	CLA	C2B-C1B	51.27	1.45	1.38
17	A	1012	CLA	C2B-C1B	51.19	1.45	1.38
17	B	1212	CLA	C2B-C1B	51.10	1.45	1.38
17	A	1901	CLA	C2B-C1B	51.09	1.45	1.38
17	Q	5224	CLA	C2B-C1B	51.04	1.45	1.38
17	P	5122	CLA	C2B-C1B	50.93	1.45	1.38
17	Q	5212	CLA	C2B-C1B	50.92	1.45	1.38
17	L	1503	CLA	C2B-C1B	50.87	1.45	1.38
17	6	5503	CLA	C2B-C1B	50.84	1.45	1.38
17	A	1132	CLA	C3B-C4B	50.83	1.45	1.38
17	Q	5214	CLA	C2B-C1B	50.81	1.45	1.38
17	B	1224	CLA	C2B-C1B	50.79	1.45	1.38
17	P	5132	CLA	C3B-C4B	50.75	1.45	1.38
17	A	1122	CLA	C2B-C1B	50.75	1.45	1.38
17	A	1011	CLA	C3B-C4B	50.72	1.45	1.38
17	P	5011	CLA	C3B-C4B	50.67	1.45	1.38
17	B	1239	CLA	C3B-C4B	50.29	1.45	1.38
17	F	1229	CLA	C2B-C1B	50.17	1.45	1.38
17	B	1214	CLA	C2B-C1B	50.16	1.45	1.38
17	Q	5239	CLA	C3B-C4B	49.99	1.45	1.38
17	U	5229	CLA	C2B-C1B	49.95	1.45	1.38
17	A	1108	CLA	C2B-C1B	49.63	1.45	1.38
17	P	5120	CLA	C2B-C1B	49.62	1.45	1.38
17	A	1120	CLA	C2B-C1B	49.49	1.45	1.38
17	B	1232	CLA	C2B-C1B	49.46	1.45	1.38
17	A	1102	CLA	C2B-C1B	49.40	1.45	1.38
17	P	5108	CLA	C2B-C1B	49.34	1.45	1.38
17	P	5102	CLA	C2B-C1B	49.23	1.45	1.38
17	A	1124	CLA	C2B-C1B	49.20	1.45	1.38
17	P	5124	CLA	C2B-C1B	48.96	1.45	1.38
17	Q	5232	CLA	C2B-C1B	48.89	1.45	1.38
17	Q	5225	CLA	C2B-C1B	48.65	1.45	1.38
17	A	1129	CLA	C2B-C1B	48.56	1.45	1.38
17	P	5129	CLA	C2B-C1B	48.21	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5206	CLA	C2B-C1B	48.20	1.45	1.38
17	B	1225	CLA	C2B-C1B	48.16	1.45	1.38
17	B	1206	CLA	C2B-C1B	47.88	1.45	1.38
17	B	1216	CLA	C2B-C1B	47.44	1.45	1.38
17	Q	5216	CLA	C2B-C1B	47.32	1.45	1.38
17	B	1237	CLA	C2B-C1B	47.12	1.45	1.38
17	Q	5237	CLA	C2B-C1B	47.04	1.45	1.38
17	P	5107	CLA	C2B-C1B	46.62	1.45	1.38
17	B	1238	CLA	C3B-C4B	45.86	1.45	1.38
17	A	1107	CLA	C2B-C1B	45.85	1.45	1.38
17	P	5011	CLA	C3D-C4D	45.82	1.45	1.38
17	Q	5238	CLA	C3B-C4B	45.59	1.45	1.38
17	A	1011	CLA	C3D-C4D	45.49	1.44	1.38
17	P	5131	CLA	C3B-C4B	44.58	1.44	1.38
17	A	1131	CLA	C3B-C4B	44.37	1.44	1.38
17	B	1022	CLA	C2B-C1B	44.23	1.44	1.38
17	Q	5022	CLA	C2B-C1B	44.22	1.44	1.38
17	B	1211	CLA	C2B-C1B	43.80	1.44	1.38
17	Q	5211	CLA	C2B-C1B	43.49	1.44	1.38
17	P	5117	CLA	C2B-C1B	43.43	1.44	1.38
17	A	1117	CLA	C2B-C1B	43.41	1.44	1.38
17	B	1206	CLA	C3B-C4B	42.21	1.44	1.38
17	Q	5206	CLA	C3B-C4B	42.05	1.44	1.38
17	A	1119	CLA	C2B-C1B	39.81	1.44	1.38
17	P	5119	CLA	C2B-C1B	39.67	1.44	1.38
17	P	5136	CLA	C2D-C1D	37.08	1.43	1.38
17	A	1136	CLA	C2D-C1D	36.84	1.43	1.38
17	L	1501	CLA	C2D-C1D	35.64	1.43	1.38
17	6	5501	CLA	C2D-C1D	35.59	1.43	1.38
17	A	1103	CLA	C2D-C1D	35.49	1.43	1.38
17	P	5103	CLA	C2D-C1D	35.26	1.43	1.38
17	Q	5211	CLA	C2D-C1D	34.47	1.43	1.38
17	B	1211	CLA	C2D-C1D	34.30	1.43	1.38
17	A	1111	CLA	C2D-C1D	34.22	1.43	1.38
17	P	5111	CLA	C2D-C1D	34.09	1.43	1.38
17	B	1209	CLA	C2D-C1D	33.23	1.43	1.38
17	Q	5235	CLA	C2D-C1D	33.14	1.43	1.38
17	B	1235	CLA	C2D-C1D	33.09	1.43	1.38
17	Q	5209	CLA	C2D-C1D	32.96	1.43	1.38
17	B	1231	CLA	C2D-C1D	32.45	1.43	1.38
17	B	1232	CLA	C2A-C1A	32.43	1.55	1.39
17	Q	5232	CLA	C2A-C1A	32.37	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5122	CLA	C2D-C1D	32.36	1.43	1.38
17	Q	5231	CLA	C2D-C1D	32.06	1.43	1.38
17	A	1122	CLA	C2D-C1D	31.88	1.43	1.38
17	P	5104	CLA	C2A-C1A	31.45	1.55	1.39
17	A	1104	CLA	C2A-C1A	31.37	1.55	1.39
17	Q	5230	CLA	C2D-C1D	31.29	1.43	1.38
17	B	1228	CLA	C2D-C1D	31.15	1.43	1.38
17	Q	5203	CLA	C2D-C1D	31.15	1.43	1.38
17	P	5012	CLA	C2A-C1A	31.03	1.55	1.39
17	B	1203	CLA	C2D-C1D	31.02	1.43	1.38
17	Q	5213	CLA	C2D-C1D	30.99	1.43	1.38
17	B	1213	CLA	C2D-C1D	30.94	1.43	1.38
17	A	1012	CLA	C2A-C1A	30.91	1.55	1.39
17	B	1230	CLA	C2D-C1D	30.81	1.43	1.38
17	Q	5228	CLA	C2D-C1D	30.80	1.43	1.38
17	Q	5221	CLA	C2A-C1A	30.79	1.54	1.39
17	B	1221	CLA	C2A-C1A	30.77	1.54	1.39
17	B	1238	CLA	C2D-C1D	30.62	1.42	1.38
17	P	5137	CLA	C2A-C1A	30.62	1.54	1.39
17	A	1137	CLA	C2A-C1A	30.58	1.54	1.39
17	B	1205	CLA	C2D-C1D	30.41	1.42	1.38
17	Q	5205	CLA	C2D-C1D	30.29	1.42	1.38
17	P	5120	CLA	C2D-C1D	30.16	1.42	1.38
17	Q	5218	CLA	C2A-C1A	30.15	1.54	1.39
17	B	1218	CLA	C2A-C1A	30.12	1.54	1.39
17	P	5129	CLA	C2D-C1D	30.07	1.42	1.38
17	A	1120	CLA	C2D-C1D	30.04	1.42	1.38
17	Q	5238	CLA	C2D-C1D	29.99	1.42	1.38
17	P	5123	CLA	C2A-C1A	29.98	1.54	1.39
17	A	1123	CLA	C2A-C1A	29.96	1.54	1.39
17	A	1901	CLA	C2A-C1A	29.91	1.54	1.39
17	Q	5208	CLA	C2D-C1D	29.88	1.42	1.38
17	P	5137	CLA	C2D-C1D	29.87	1.42	1.38
17	A	1129	CLA	C2D-C1D	29.84	1.42	1.38
17	B	1208	CLA	C2D-C1D	29.80	1.42	1.38
17	P	5901	CLA	C2A-C1A	29.77	1.54	1.39
17	A	1122	CLA	C2A-C1A	29.75	1.54	1.39
17	P	5122	CLA	C2A-C1A	29.75	1.54	1.39
17	Q	5219	CLA	C2D-C1D	29.74	1.42	1.38
17	Q	5227	CLA	C2D-C1D	29.73	1.42	1.38
17	B	1227	CLA	C2D-C1D	29.67	1.42	1.38
17	P	5112	CLA	C2A-C1A	29.66	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1112	CLA	C2A-C1A	29.62	1.54	1.39
17	B	1210	CLA	C2D-C1D	29.60	1.42	1.38
17	Q	5216	CLA	C2A-C1A	29.56	1.54	1.39
17	P	5107	CLA	C2A-C1A	29.54	1.54	1.39
17	Z	5302	CLA	C2A-C1A	29.54	1.54	1.39
17	A	1107	CLA	C2A-C1A	29.47	1.54	1.39
17	B	1219	CLA	C2D-C1D	29.47	1.42	1.38
17	K	1401	CLA	C2A-C1A	29.44	1.54	1.39
17	B	1216	CLA	C2A-C1A	29.38	1.54	1.39
17	J	1302	CLA	C2A-C1A	29.37	1.54	1.39
17	5	5401	CLA	C2A-C1A	29.31	1.54	1.39
17	Q	5206	CLA	C2A-C1A	29.29	1.54	1.39
17	Q	5223	CLA	C2A-C1A	29.27	1.54	1.39
17	B	1214	CLA	C2A-C1A	29.26	1.54	1.39
17	B	1223	CLA	C2A-C1A	29.25	1.54	1.39
17	B	1206	CLA	C2A-C1A	29.23	1.54	1.39
17	B	1238	CLA	C2A-C1A	29.19	1.54	1.39
17	Q	5214	CLA	C2A-C1A	29.19	1.54	1.39
17	A	1135	CLA	C2A-C1A	29.18	1.54	1.39
17	Q	5238	CLA	C2A-C1A	29.17	1.54	1.39
17	P	5139	CLA	C2A-C1A	29.16	1.54	1.39
17	A	1139	CLA	C2A-C1A	29.14	1.54	1.39
17	A	1137	CLA	C2D-C1D	29.14	1.42	1.38
17	A	1105	CLA	C2A-C1A	29.08	1.54	1.39
17	P	5102	CLA	C2A-C1A	29.07	1.54	1.39
17	B	1202	CLA	C2D-C1D	29.07	1.42	1.38
17	P	5135	CLA	C2A-C1A	29.05	1.54	1.39
17	A	1102	CLA	C2A-C1A	29.04	1.54	1.39
17	P	5105	CLA	C2A-C1A	28.97	1.54	1.39
17	Q	5220	CLA	C2A-C1A	28.97	1.54	1.39
17	B	1220	CLA	C2A-C1A	28.96	1.54	1.39
17	P	5138	CLA	C2A-C1A	28.96	1.54	1.39
17	B	1207	CLA	C2A-C1A	28.96	1.54	1.39
17	Q	5210	CLA	C2D-C1D	28.95	1.42	1.38
17	Q	5202	CLA	C2D-C1D	28.95	1.42	1.38
17	P	5110	CLA	C2A-C1A	28.91	1.53	1.39
17	A	1110	CLA	C2A-C1A	28.90	1.53	1.39
17	Q	5207	CLA	C2A-C1A	28.89	1.53	1.39
17	A	1138	CLA	C2A-C1A	28.88	1.53	1.39
17	F	1229	CLA	C2D-C1D	28.67	1.42	1.38
17	U	5229	CLA	C2D-C1D	28.63	1.42	1.38
17	6	5502	CLA	C2A-C1A	28.62	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	1502	CLA	C2A-C1A	28.52	1.53	1.39
17	A	1138	CLA	C2D-C1D	28.51	1.42	1.38
17	F	1301	CLA	C2A-C1A	28.46	1.53	1.39
17	A	1111	CLA	C2A-C1A	28.46	1.53	1.39
17	P	5111	CLA	C2A-C1A	28.46	1.53	1.39
17	U	5301	CLA	C2A-C1A	28.45	1.53	1.39
17	K	1401	CLA	C2D-C1D	28.40	1.42	1.38
17	G	1233	CLA	C2A-C1A	28.39	1.53	1.39
17	V	5233	CLA	C2A-C1A	28.38	1.53	1.39
17	B	1221	CLA	C2D-C1D	28.32	1.42	1.38
17	A	1113	CLA	C2D-C1D	28.26	1.42	1.38
17	Q	5221	CLA	C2D-C1D	28.26	1.42	1.38
17	A	1112	CLA	C2D-C1D	28.23	1.42	1.38
17	P	5113	CLA	C2D-C1D	28.20	1.42	1.38
17	B	1211	CLA	C2A-C1A	28.19	1.53	1.39
17	Q	5211	CLA	C2A-C1A	28.18	1.53	1.39
17	Q	5234	CLA	C2A-C1A	28.17	1.53	1.39
17	Q	5236	CLA	C2A-C1A	28.16	1.53	1.39
17	B	1234	CLA	C2A-C1A	28.15	1.53	1.39
17	B	1236	CLA	C2A-C1A	28.11	1.53	1.39
17	P	5134	CLA	C2A-C1A	28.10	1.53	1.39
17	A	1116	CLA	C2A-C1A	28.10	1.53	1.39
17	P	5135	CLA	C2D-C1D	28.09	1.42	1.38
17	Q	5210	CLA	C2A-C1A	28.08	1.53	1.39
17	Q	5023	CLA	C2D-C1D	28.07	1.42	1.38
17	B	1208	CLA	C2A-C1A	28.04	1.53	1.39
17	A	1135	CLA	C2D-C1D	28.03	1.42	1.38
17	A	1134	CLA	C2A-C1A	28.03	1.53	1.39
17	5	5401	CLA	C2D-C1D	28.01	1.42	1.38
17	B	1217	CLA	C2A-C1A	27.99	1.53	1.39
17	P	5138	CLA	C2D-C1D	27.98	1.42	1.38
17	P	5115	CLA	C2D-C1D	27.97	1.42	1.38
17	Q	5217	CLA	C2A-C1A	27.96	1.53	1.39
17	Q	5213	CLA	C2A-C1A	27.96	1.53	1.39
17	P	5116	CLA	C2A-C1A	27.95	1.53	1.39
17	Q	5208	CLA	C2A-C1A	27.93	1.53	1.39
17	B	1210	CLA	C2A-C1A	27.92	1.53	1.39
17	B	1213	CLA	C2A-C1A	27.87	1.53	1.39
17	6	5503	CLA	C2D-C1D	27.83	1.42	1.38
17	P	5112	CLA	C2D-C1D	27.75	1.42	1.38
17	A	1115	CLA	C2D-C1D	27.73	1.42	1.38
17	P	5127	CLA	C2A-C1A	27.72	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5130	CLA	C2A-C1A	27.69	1.53	1.39
17	B	1130	CLA	C2A-C1A	27.69	1.53	1.39
17	P	5113	CLA	C2A-C1A	27.67	1.53	1.39
17	B	1212	CLA	C2A-C1A	27.64	1.53	1.39
17	A	1113	CLA	C2A-C1A	27.63	1.53	1.39
17	B	1239	CLA	C2D-C1D	27.62	1.42	1.38
17	A	1127	CLA	C2A-C1A	27.61	1.53	1.39
17	A	1121	CLA	C2A-C1A	27.59	1.53	1.39
17	P	5121	CLA	C2A-C1A	27.59	1.53	1.39
17	Q	5212	CLA	C2A-C1A	27.57	1.53	1.39
17	P	5402	CLA	C2A-C1A	27.57	1.53	1.39
17	A	1402	CLA	C2A-C1A	27.51	1.53	1.39
17	Q	5239	CLA	C2D-C1D	27.50	1.42	1.38
17	A	1134	CLA	C2D-C1D	27.47	1.42	1.38
17	8	1015	CLA	C2A-C1A	27.45	1.53	1.39
17	Q	5231	CLA	C2A-C1A	27.44	1.53	1.39
17	P	5118	CLA	C2A-C1A	27.44	1.53	1.39
17	A	1118	CLA	C2A-C1A	27.43	1.53	1.39
17	2	1015	CLA	C2A-C1A	27.43	1.53	1.39
17	B	1231	CLA	C2A-C1A	27.39	1.53	1.39
17	A	1119	CLA	C2A-C1A	27.39	1.53	1.39
17	P	5134	CLA	C2D-C1D	27.38	1.42	1.38
17	P	5119	CLA	C2A-C1A	27.37	1.53	1.39
17	Q	5226	CLA	C2A-C1A	27.37	1.53	1.39
17	Q	5224	CLA	C2D-C1D	27.36	1.42	1.38
17	7	1026	CLA	C2A-C1A	27.36	1.53	1.39
17	B	1226	CLA	C2A-C1A	27.35	1.53	1.39
17	0	1022	CLA	C2A-C1A	27.34	1.53	1.39
17	B	1023	CLA	C2D-C1D	27.34	1.42	1.38
17	0	8002	CLA	C2A-C1A	27.32	1.53	1.39
17	9	1011	CLA	C2A-C1A	27.32	1.53	1.39
17	Z	8008	CLA	C2A-C1A	27.32	1.53	1.39
17	A	1120	CLA	C2A-C1A	27.31	1.53	1.39
17	P	5120	CLA	C2A-C1A	27.30	1.53	1.39
17	L	1503	CLA	C2D-C1D	27.30	1.42	1.38
17	4	1031	CLA	C2A-C1A	27.29	1.53	1.39
17	P	5128	CLA	C2A-C1A	27.29	1.53	1.39
17	8	1017	CLA	C2A-C1A	27.29	1.53	1.39
17	Q	5242	CLA	C2A-C1A	27.28	1.53	1.39
17	2	1022	CLA	C2A-C1A	27.28	1.53	1.39
17	9	1014	CLA	C2A-C1A	27.27	1.53	1.39
17	H	1801	CLA	C2A-C1A	27.27	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	1014	CLA	C2A-C1A	27.26	1.53	1.39
17	5	5404	CLA	C2A-C1A	27.26	1.53	1.39
17	J	4008	CLA	C2A-C1A	27.25	1.53	1.39
17	B	1220	CLA	C2D-C1D	27.24	1.42	1.38
17	8	1022	CLA	C2A-C1A	27.24	1.53	1.39
17	U	8004	CLA	C2A-C1A	27.24	1.53	1.39
17	2	1014	CLA	C2A-C1A	27.23	1.53	1.39
17	3	1031	CLA	C2A-C1A	27.23	1.53	1.39
17	W	5801	CLA	C2A-C1A	27.23	1.53	1.39
17	4	1022	CLA	C2A-C1A	27.22	1.53	1.39
17	8	1023	CLA	C2A-C1A	27.22	1.53	1.39
17	A	1128	CLA	C2A-C1A	27.22	1.53	1.39
17	3	1011	CLA	C2A-C1A	27.22	1.53	1.39
17	4	1016	CLA	C2A-C1A	27.22	1.53	1.39
17	1	1026	CLA	C2A-C1A	27.22	1.53	1.39
17	0	1032	CLA	C2A-C1A	27.22	1.53	1.39
17	B	1224	CLA	C2D-C1D	27.22	1.42	1.38
17	F	4004	CLA	C2A-C1A	27.20	1.53	1.39
17	3	1022	CLA	C2A-C1A	27.20	1.53	1.39
17	2	1017	CLA	C2A-C1A	27.20	1.53	1.39
17	4	1026	CLA	C2A-C1A	27.19	1.53	1.39
17	P	8009	CLA	C2A-C1A	27.19	1.53	1.39
17	4	1017	CLA	C2A-C1A	27.18	1.53	1.39
17	Q	5220	CLA	C2D-C1D	27.19	1.42	1.38
17	9	1026	CLA	C2A-C1A	27.18	1.53	1.39
17	A	4009	CLA	C2A-C1A	27.18	1.53	1.39
17	Z	5101	CLA	C2A-C1A	27.18	1.53	1.39
17	U	8005	CLA	C2A-C1A	27.18	1.53	1.39
17	9	1022	CLA	C2A-C1A	27.18	1.53	1.39
17	4	1025	CLA	C2A-C1A	27.17	1.53	1.39
17	V	5701	CLA	C2A-C1A	27.17	1.53	1.39
17	0	1031	CLA	C2A-C1A	27.17	1.53	1.39
17	3	1014	CLA	C2A-C1A	27.16	1.53	1.39
17	K	1403	CLA	C2A-C1A	27.16	1.53	1.39
17	7	1031	CLA	C2A-C1A	27.16	1.53	1.39
17	4	4002	CLA	C2A-C1A	27.16	1.53	1.39
17	B	1240	CLA	C2A-C1A	27.16	1.53	1.39
17	6	5504	CLA	C2A-C1A	27.15	1.53	1.39
17	7	1025	CLA	C2A-C1A	27.15	1.53	1.39
17	1	1025	CLA	C2A-C1A	27.15	1.53	1.39
17	K	1404	CLA	C2A-C1A	27.15	1.53	1.39
17	0	1026	CLA	C2A-C1A	27.15	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	4010	CLA	C2A-C1A	27.15	1.53	1.39
17	P	8010	CLA	C2A-C1A	27.15	1.53	1.39
17	7	1012	CLA	C2A-C1A	27.14	1.53	1.39
17	0	1016	CLA	C2A-C1A	27.14	1.53	1.39
17	1	1031	CLA	C2A-C1A	27.14	1.53	1.39
17	F	4005	CLA	C2A-C1A	27.13	1.53	1.39
17	4	1012	CLA	C2A-C1A	27.13	1.53	1.39
17	0	1014	CLA	C2A-C1A	27.13	1.53	1.39
17	1	1021	CLA	C2A-C1A	27.13	1.53	1.39
17	J	1101	CLA	C2A-C1A	27.13	1.53	1.39
17	7	1016	CLA	C2A-C1A	27.13	1.53	1.39
17	2	1023	CLA	C2A-C1A	27.13	1.53	1.39
17	Q	5240	CLA	C2A-C1A	27.13	1.53	1.39
17	7	1021	CLA	C2A-C1A	27.12	1.53	1.39
17	7	1017	CLA	C2A-C1A	27.12	1.53	1.39
17	G	1701	CLA	C2A-C1A	27.12	1.53	1.39
17	1	1011	CLA	C2A-C1A	27.12	1.53	1.39
17	4	1011	CLA	C2A-C1A	27.12	1.53	1.39
17	4	1021	CLA	C2A-C1A	27.12	1.53	1.39
17	7	1011	CLA	C2A-C1A	27.11	1.53	1.39
17	4	1014	CLA	C2A-C1A	27.11	1.53	1.39
17	0	1025	CLA	C2A-C1A	27.11	1.53	1.39
17	0	1017	CLA	C2A-C1A	27.11	1.53	1.39
17	A	1114	CLA	C2A-C1A	27.11	1.53	1.39
17	0	1011	CLA	C2A-C1A	27.11	1.53	1.39
17	3	1026	CLA	C2A-C1A	27.11	1.53	1.39
17	F	4003	CLA	C2A-C1A	27.10	1.53	1.39
17	7	1022	CLA	C2A-C1A	27.10	1.53	1.39
17	0	1021	CLA	C2A-C1A	27.10	1.53	1.39
17	P	5114	CLA	C2A-C1A	27.10	1.53	1.39
17	4	1032	CLA	C2A-C1A	27.09	1.53	1.39
17	0	1033	CLA	C2A-C1A	27.09	1.53	1.39
17	Q	8001	CLA	C2A-C1A	27.09	1.53	1.39
17	B	1242	CLA	C2A-C1A	27.09	1.53	1.39
17	A	1125	CLA	C2A-C1A	27.09	1.53	1.39
17	L	1504	CLA	C2A-C1A	27.08	1.53	1.39
17	2	4007	CLA	C2A-C1A	27.08	1.53	1.39
17	8	1013	CLA	C2A-C1A	27.08	1.53	1.39
17	9	1031	CLA	C2A-C1A	27.08	1.53	1.39
17	1	1017	CLA	C2A-C1A	27.08	1.53	1.39
17	2	1025	CLA	C2A-C1A	27.08	1.53	1.39
17	2	1016	CLA	C2A-C1A	27.08	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	1012	CLA	C2A-C1A	27.08	1.53	1.39
17	1	1016	CLA	C2A-C1A	27.07	1.53	1.39
17	4	1033	CLA	C2A-C1A	27.07	1.53	1.39
17	2	1026	CLA	C2A-C1A	27.07	1.53	1.39
17	F	4006	CLA	C2A-C1A	27.07	1.53	1.39
17	B	1241	CLA	C2A-C1A	27.07	1.53	1.39
17	2	1011	CLA	C2A-C1A	27.07	1.53	1.39
17	7	1013	CLA	C2A-C1A	27.06	1.53	1.39
17	B	4001	CLA	C2A-C1A	27.06	1.53	1.39
17	8	1012	CLA	C2A-C1A	27.06	1.53	1.39
17	1	1023	CLA	C2A-C1A	27.06	1.53	1.39
17	8	1025	CLA	C2A-C1A	27.06	1.53	1.39
17	1	1013	CLA	C2A-C1A	27.05	1.53	1.39
17	1	1012	CLA	C2A-C1A	27.04	1.53	1.39
17	Q	5241	CLA	C2A-C1A	27.04	1.53	1.39
17	P	5125	CLA	C2A-C1A	27.04	1.53	1.39
17	8	1016	CLA	C2A-C1A	27.04	1.53	1.39
17	2	1013	CLA	C2A-C1A	27.04	1.53	1.39
17	1	1022	CLA	C2A-C1A	27.03	1.53	1.39
17	6	5501	CLA	C2A-C1A	27.03	1.53	1.39
17	7	1015	CLA	C2A-C1A	27.02	1.53	1.39
17	2	1012	CLA	C2A-C1A	27.02	1.53	1.39
17	7	1023	CLA	C2A-C1A	27.02	1.53	1.39
17	9	1032	CLA	C2A-C1A	27.02	1.53	1.39
17	8	1026	CLA	C2A-C1A	27.01	1.53	1.39
17	5	5403	CLA	C2A-C1A	27.01	1.53	1.39
17	3	1041	CLA	C2A-C1A	27.01	1.53	1.39
17	0	1013	CLA	C2A-C1A	27.00	1.53	1.39
17	3	1033	CLA	C2A-C1A	27.00	1.53	1.39
17	0	1012	CLA	C2A-C1A	26.99	1.52	1.39
17	8	8007	CLA	C2A-C1A	26.99	1.52	1.39
17	2	1031	CLA	C2A-C1A	26.99	1.52	1.39
17	3	1032	CLA	C2A-C1A	26.99	1.52	1.39
17	L	1501	CLA	C2A-C1A	26.98	1.52	1.39
17	3	1012	CLA	C2A-C1A	26.98	1.52	1.39
17	3	1015	CLA	C2A-C1A	26.98	1.52	1.39
17	2	1033	CLA	C2A-C1A	26.98	1.52	1.39
17	U	8006	CLA	C2A-C1A	26.97	1.52	1.39
17	Q	5237	CLA	C2D-C1D	26.97	1.42	1.38
17	8	1011	CLA	C2A-C1A	26.96	1.52	1.39
17	9	1033	CLA	C2A-C1A	26.96	1.52	1.39
17	4	1015	CLA	C2A-C1A	26.95	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	1031	CLA	C2A-C1A	26.95	1.52	1.39
17	U	8003	CLA	C2A-C1A	26.95	1.52	1.39
17	1	1015	CLA	C2A-C1A	26.94	1.52	1.39
17	0	1015	CLA	C2A-C1A	26.93	1.52	1.39
17	3	1017	CLA	C2A-C1A	26.93	1.52	1.39
17	9	1016	CLA	C2A-C1A	26.93	1.52	1.39
17	4	1023	CLA	C2A-C1A	26.92	1.52	1.39
17	9	1041	CLA	C2A-C1A	26.92	1.52	1.39
17	1	1014	CLA	C2A-C1A	26.91	1.52	1.39
17	7	1014	CLA	C2A-C1A	26.89	1.52	1.39
17	4	1013	CLA	C2A-C1A	26.89	1.52	1.39
17	3	1016	CLA	C2A-C1A	26.89	1.52	1.39
17	8	1021	CLA	C2A-C1A	26.89	1.52	1.39
17	9	1015	CLA	C2A-C1A	26.87	1.52	1.39
17	9	1025	CLA	C2A-C1A	26.87	1.52	1.39
17	8	1033	CLA	C2A-C1A	26.85	1.52	1.39
17	3	1025	CLA	C2A-C1A	26.84	1.52	1.39
17	2	1021	CLA	C2A-C1A	26.82	1.52	1.39
17	3	1021	CLA	C2A-C1A	26.79	1.52	1.39
17	9	1017	CLA	C2A-C1A	26.77	1.52	1.39
17	B	1237	CLA	C2D-C1D	26.75	1.42	1.38
17	0	1023	CLA	C2A-C1A	26.76	1.52	1.39
17	9	1021	CLA	C2A-C1A	26.73	1.52	1.39
17	A	1108	CLA	C2A-C1A	26.66	1.52	1.39
17	Q	5201	CLA	C2A-C1A	26.66	1.52	1.39
17	A	1013	CLA	C2A-C1A	26.64	1.52	1.39
17	P	5126	CLA	C2D-C1D	26.63	1.42	1.38
17	P	5108	CLA	C2A-C1A	26.61	1.52	1.39
17	Q	5205	CLA	C2A-C1A	26.58	1.52	1.39
17	B	1201	CLA	C2A-C1A	26.56	1.52	1.39
17	P	5013	CLA	C2A-C1A	26.52	1.52	1.39
17	P	5118	CLA	C2D-C1D	26.50	1.42	1.38
17	A	1140	CLA	C2A-C1A	26.49	1.52	1.39
17	P	5140	CLA	C2A-C1A	26.47	1.52	1.39
17	B	1205	CLA	C2A-C1A	26.46	1.52	1.39
17	A	1135	CLA	C3D-C4D	26.42	1.42	1.38
17	P	5117	CLA	C2A-C1A	26.39	1.52	1.39
17	P	5135	CLA	C3D-C4D	26.38	1.42	1.38
17	A	1117	CLA	C2A-C1A	26.37	1.52	1.39
17	A	1011	CLA	C2A-C1A	26.36	1.52	1.39
17	A	1118	CLA	C2D-C1D	26.35	1.42	1.38
17	Q	5023	CLA	C2A-C1A	26.30	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5011	CLA	C2A-C1A	26.29	1.52	1.39
17	Q	5209	CLA	C2A-C1A	26.29	1.52	1.39
17	Q	5219	CLA	C2A-C1A	26.28	1.52	1.39
17	B	1219	CLA	C2A-C1A	26.24	1.52	1.39
17	A	1126	CLA	C2D-C1D	26.21	1.42	1.38
17	P	5121	CLA	C2D-C1D	26.18	1.42	1.38
17	B	1023	CLA	C2A-C1A	26.17	1.52	1.39
17	B	1209	CLA	C2A-C1A	26.15	1.52	1.39
17	P	5115	CLA	C2A-C1A	26.14	1.52	1.39
17	A	1115	CLA	C2A-C1A	26.14	1.52	1.39
17	P	5129	CLA	C2A-C1A	26.06	1.52	1.39
17	A	1129	CLA	C2A-C1A	26.04	1.52	1.39
17	A	1121	CLA	C2D-C1D	25.97	1.42	1.38
17	Q	5204	CLA	C2A-C1A	25.96	1.52	1.39
17	B	1204	CLA	C2A-C1A	25.91	1.52	1.39
17	A	1126	CLA	C2A-C1A	25.78	1.52	1.39
17	P	5126	CLA	C2A-C1A	25.75	1.52	1.39
17	Q	5222	CLA	C2A-C1A	25.72	1.52	1.39
17	A	1106	CLA	C2A-C1A	25.71	1.52	1.39
17	B	1218	CLA	C2D-C1D	25.71	1.42	1.38
17	B	1222	CLA	C2A-C1A	25.67	1.52	1.39
17	P	5131	CLA	C2D-C1D	25.64	1.42	1.38
17	P	5106	CLA	C2A-C1A	25.63	1.52	1.39
17	P	5106	CLA	C2D-C1D	25.60	1.42	1.38
17	B	1215	CLA	C2D-C1D	25.51	1.42	1.38
17	B	1203	CLA	C2A-C1A	25.47	1.52	1.39
17	B	1228	CLA	C2A-C1A	25.43	1.52	1.39
17	Q	5203	CLA	C2A-C1A	25.39	1.52	1.39
17	Q	5218	CLA	C2D-C1D	25.39	1.42	1.38
17	Q	5228	CLA	C2A-C1A	25.38	1.52	1.39
17	P	5124	CLA	C2D-C1D	25.37	1.42	1.38
17	B	1225	CLA	C2A-C1A	25.32	1.52	1.39
17	A	1114	CLA	C2D-C1D	25.32	1.42	1.38
17	B	1023	CLA	C3D-C4D	25.28	1.42	1.38
17	A	1131	CLA	C2D-C1D	25.27	1.42	1.38
17	A	1106	CLA	C2D-C1D	25.26	1.42	1.38
17	P	5108	CLA	C2D-C1D	25.24	1.42	1.38
17	A	1133	CLA	C2A-C1A	25.21	1.52	1.39
17	P	5133	CLA	C2A-C1A	25.21	1.52	1.39
17	Q	5225	CLA	C2A-C1A	25.18	1.52	1.39
17	B	1227	CLA	C2A-C1A	25.17	1.52	1.39
17	A	1124	CLA	C2D-C1D	25.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5136	CLA	C2A-C1A	25.12	1.52	1.39
17	Q	5227	CLA	C2A-C1A	25.09	1.52	1.39
17	6	5503	CLA	C2A-C1A	25.06	1.52	1.39
17	A	1136	CLA	C2A-C1A	25.05	1.52	1.39
17	P	5114	CLA	C2D-C1D	24.99	1.42	1.38
17	L	1503	CLA	C2A-C1A	24.99	1.51	1.39
17	Q	5215	CLA	C2D-C1D	24.98	1.42	1.38
17	P	5109	CLA	C2A-C1A	24.97	1.51	1.39
17	B	1226	CLA	C2D-C1D	24.97	1.42	1.38
17	Q	5023	CLA	C3D-C4D	24.97	1.42	1.38
17	Q	5226	CLA	C2D-C1D	24.96	1.42	1.38
17	P	5140	CLA	C2D-C1D	24.88	1.42	1.38
17	Q	5022	CLA	C2A-C1A	24.86	1.51	1.39
17	A	1140	CLA	C2D-C1D	24.85	1.42	1.38
17	A	1109	CLA	C2A-C1A	24.84	1.51	1.39
17	B	1022	CLA	C2A-C1A	24.82	1.51	1.39
17	Q	5224	CLA	C2A-C1A	24.71	1.51	1.39
17	A	1125	CLA	C2D-C1D	24.66	1.42	1.38
17	P	5125	CLA	C2D-C1D	24.62	1.42	1.38
17	P	5013	CLA	C2D-C1D	24.62	1.42	1.38
17	B	1224	CLA	C2A-C1A	24.62	1.51	1.39
17	Q	5230	CLA	C2A-C1A	24.61	1.51	1.39
17	6	5502	CLA	C2D-C1D	24.59	1.42	1.38
17	B	1239	CLA	C2A-C1A	24.50	1.51	1.39
17	Q	5239	CLA	C2A-C1A	24.45	1.51	1.39
17	B	1230	CLA	C2A-C1A	24.44	1.51	1.39
17	9	1021	CLA	C2D-C1D	24.42	1.42	1.38
17	A	1110	CLA	C3D-C4D	24.41	1.42	1.38
17	8	1014	CLA	C2D-C1D	24.40	1.42	1.38
17	A	1108	CLA	C2D-C1D	24.39	1.42	1.38
17	B	1201	CLA	C2D-C1D	24.35	1.42	1.38
17	L	1502	CLA	C2D-C1D	24.35	1.42	1.38
17	Q	5234	CLA	C2D-C1D	24.33	1.42	1.38
17	B	1234	CLA	C2D-C1D	24.32	1.42	1.38
17	P	5110	CLA	C3D-C4D	24.27	1.42	1.38
17	2	1014	CLA	C2D-C1D	24.20	1.42	1.38
17	Q	5201	CLA	C2D-C1D	24.18	1.42	1.38
17	3	1021	CLA	C2D-C1D	24.16	1.42	1.38
17	A	1013	CLA	C2D-C1D	24.14	1.42	1.38
17	P	5131	CLA	C2A-C1A	24.14	1.51	1.39
17	Q	5215	CLA	C2A-C1A	24.14	1.51	1.39
17	A	1124	CLA	C2A-C1A	24.10	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	1021	CLA	C2D-C1D	24.08	1.42	1.38
17	B	1215	CLA	C2A-C1A	24.07	1.51	1.39
17	A	1131	CLA	C2A-C1A	24.05	1.51	1.39
17	P	5124	CLA	C2A-C1A	24.04	1.51	1.39
17	B	1235	CLA	C2A-C1A	24.01	1.51	1.39
17	3	1015	CLA	C2D-C1D	23.98	1.42	1.38
17	9	1033	CLA	C2D-C1D	23.97	1.42	1.38
17	Q	5235	CLA	C2A-C1A	23.94	1.51	1.39
17	P	8010	CLA	C2D-C1D	23.93	1.42	1.38
17	Z	8008	CLA	C2D-C1D	23.93	1.42	1.38
17	1	1021	CLA	C2D-C1D	23.92	1.42	1.38
17	9	1016	CLA	C2D-C1D	23.92	1.42	1.38
17	7	1014	CLA	C2D-C1D	23.89	1.42	1.38
17	7	1022	CLA	C2D-C1D	23.87	1.42	1.38
17	0	1023	CLA	C2D-C1D	23.87	1.42	1.38
17	0	1022	CLA	C2D-C1D	23.86	1.42	1.38
17	2	1031	CLA	C2D-C1D	23.85	1.42	1.38
17	8	1031	CLA	C2D-C1D	23.81	1.42	1.38
17	3	1016	CLA	C2D-C1D	23.81	1.42	1.38
17	9	1011	CLA	C2D-C1D	23.80	1.42	1.38
17	4	1013	CLA	C2D-C1D	23.76	1.42	1.38
17	0	1032	CLA	C2D-C1D	23.70	1.42	1.38
17	F	1229	CLA	C2A-C1A	23.70	1.51	1.39
17	U	5229	CLA	C2A-C1A	23.69	1.51	1.39
17	4	1015	CLA	C2D-C1D	23.67	1.42	1.38
17	8	1016	CLA	C2D-C1D	23.66	1.42	1.38
17	A	1123	CLA	C2D-C1D	23.66	1.42	1.38
17	U	8005	CLA	C2D-C1D	23.65	1.42	1.38
17	4	1011	CLA	C2D-C1D	23.65	1.42	1.38
17	P	5107	CLA	C2D-C1D	23.64	1.42	1.38
17	Q	5225	CLA	C2D-C1D	23.64	1.42	1.38
17	2	1011	CLA	C2D-C1D	23.64	1.42	1.38
17	1	1022	CLA	C2D-C1D	23.64	1.42	1.38
17	1	1014	CLA	C2D-C1D	23.63	1.42	1.38
17	8	1011	CLA	C2D-C1D	23.63	1.42	1.38
17	9	1015	CLA	C2D-C1D	23.62	1.42	1.38
17	F	4005	CLA	C2D-C1D	23.62	1.42	1.38
17	W	5801	CLA	C2D-C1D	23.62	1.42	1.38
17	7	1012	CLA	C2D-C1D	23.61	1.42	1.38
17	A	4010	CLA	C2D-C1D	23.61	1.42	1.38
17	0	1026	CLA	C2D-C1D	23.59	1.42	1.38
17	0	1013	CLA	C2D-C1D	23.58	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	0	1017	CLA	C2D-C1D	23.57	1.42	1.38
17	2	1033	CLA	C2D-C1D	23.57	1.42	1.38
17	3	1011	CLA	C2D-C1D	23.56	1.42	1.38
17	0	1016	CLA	C2D-C1D	23.56	1.42	1.38
17	1	1013	CLA	C2D-C1D	23.56	1.42	1.38
17	1	1012	CLA	C2D-C1D	23.55	1.42	1.38
17	3	1025	CLA	C2D-C1D	23.53	1.42	1.38
17	4	4002	CLA	C2D-C1D	23.52	1.42	1.38
17	J	4008	CLA	C2D-C1D	23.48	1.42	1.38
17	3	1031	CLA	C2D-C1D	23.47	1.42	1.38
17	P	5117	CLA	C2D-C1D	23.46	1.42	1.38
17	Q	5021	CLA	C3D-C4D	23.45	1.42	1.38
17	4	1023	CLA	C2D-C1D	23.45	1.42	1.38
17	B	1225	CLA	C2D-C1D	23.44	1.42	1.38
17	2	1023	CLA	C2D-C1D	23.42	1.42	1.38
17	U	8003	CLA	C2D-C1D	23.41	1.42	1.38
17	7	1013	CLA	C2D-C1D	23.41	1.42	1.38
17	H	1801	CLA	C2D-C1D	23.40	1.42	1.38
17	Q	5242	CLA	C2D-C1D	23.39	1.42	1.38
17	A	1117	CLA	C2D-C1D	23.38	1.42	1.38
17	9	1031	CLA	C2D-C1D	23.38	1.42	1.38
17	Z	5101	CLA	C2D-C1D	23.37	1.42	1.38
17	B	1021	CLA	C2A-C1A	23.37	1.51	1.39
17	7	1023	CLA	C2D-C1D	23.36	1.42	1.38
17	4	1032	CLA	C2D-C1D	23.35	1.42	1.38
17	Q	5021	CLA	C2A-C1A	23.34	1.51	1.39
17	0	8002	CLA	C2D-C1D	23.33	1.42	1.38
17	F	4004	CLA	C2D-C1D	23.32	1.42	1.38
17	B	1242	CLA	C2D-C1D	23.32	1.42	1.38
17	B	1240	CLA	C2D-C1D	23.32	1.42	1.38
17	8	1025	CLA	C2D-C1D	23.32	1.42	1.38
17	0	1015	CLA	C2D-C1D	23.32	1.42	1.38
17	9	1025	CLA	C2D-C1D	23.31	1.42	1.38
17	4	1016	CLA	C2D-C1D	23.30	1.42	1.38
17	8	1022	CLA	C2D-C1D	23.30	1.42	1.38
17	3	1033	CLA	C2D-C1D	23.29	1.42	1.38
17	9	1026	CLA	C2D-C1D	23.29	1.42	1.38
17	P	5123	CLA	C2D-C1D	23.29	1.42	1.38
17	Z	5302	CLA	C2D-C1D	23.28	1.42	1.38
17	5	5404	CLA	C2D-C1D	23.26	1.41	1.38
17	2	1016	CLA	C2D-C1D	23.25	1.41	1.38
17	Q	8001	CLA	C2D-C1D	23.23	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	1033	CLA	C2D-C1D	23.23	1.41	1.38
17	3	1026	CLA	C2D-C1D	23.23	1.41	1.38
17	1	1023	CLA	C2D-C1D	23.22	1.41	1.38
17	1	1016	CLA	C2D-C1D	23.22	1.41	1.38
17	F	4006	CLA	C2D-C1D	23.21	1.41	1.38
17	J	1302	CLA	C2D-C1D	23.21	1.41	1.38
17	4	1025	CLA	C2D-C1D	23.20	1.41	1.38
17	1	1025	CLA	C2D-C1D	23.20	1.41	1.38
17	5	5403	CLA	C2D-C1D	23.19	1.41	1.38
17	J	1101	CLA	C2D-C1D	23.18	1.41	1.38
17	B	1021	CLA	C3D-C4D	23.18	1.41	1.38
17	K	1403	CLA	C2D-C1D	23.18	1.41	1.38
17	1	1017	CLA	C2D-C1D	23.18	1.41	1.38
17	2	1022	CLA	C2D-C1D	23.17	1.41	1.38
17	A	1119	CLA	C2D-C1D	23.16	1.41	1.38
17	4	1012	CLA	C2D-C1D	23.16	1.41	1.38
17	9	1017	CLA	C2D-C1D	23.16	1.41	1.38
17	4	1022	CLA	C2D-C1D	23.16	1.41	1.38
17	4	1033	CLA	C2D-C1D	23.16	1.41	1.38
17	4	1026	CLA	C2D-C1D	23.15	1.41	1.38
17	6	5504	CLA	C2D-C1D	23.15	1.41	1.38
17	3	1017	CLA	C2D-C1D	23.14	1.41	1.38
17	7	1025	CLA	C2D-C1D	23.13	1.41	1.38
17	P	5103	CLA	C2A-C1A	23.13	1.51	1.39
17	4	1021	CLA	C2D-C1D	23.13	1.41	1.38
17	A	1107	CLA	C2D-C1D	23.12	1.41	1.38
17	2	1017	CLA	C2D-C1D	23.12	1.41	1.38
17	8	1015	CLA	C2D-C1D	23.12	1.41	1.38
17	B	4001	CLA	C2D-C1D	23.10	1.41	1.38
17	2	1025	CLA	C2D-C1D	23.09	1.41	1.38
17	L	1504	CLA	C2D-C1D	23.09	1.41	1.38
17	0	1011	CLA	C2D-C1D	23.09	1.41	1.38
17	A	1103	CLA	C2A-C1A	23.08	1.50	1.39
17	2	1015	CLA	C2D-C1D	23.07	1.41	1.38
17	7	1016	CLA	C2D-C1D	23.07	1.41	1.38
17	8	1026	CLA	C2D-C1D	23.07	1.41	1.38
17	7	1017	CLA	C2D-C1D	23.06	1.41	1.38
17	0	1021	CLA	C2D-C1D	23.06	1.41	1.38
17	Q	5240	CLA	C2D-C1D	23.06	1.41	1.38
17	2	1026	CLA	C2D-C1D	23.06	1.41	1.38
17	K	1404	CLA	C2D-C1D	23.03	1.41	1.38
17	U	8004	CLA	C2D-C1D	23.01	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	1041	CLA	C2D-C1D	23.01	1.41	1.38
17	P	5132	CLA	C2A-C1A	23.00	1.50	1.39
17	A	1132	CLA	C2A-C1A	23.00	1.50	1.39
17	8	1023	CLA	C2D-C1D	23.00	1.41	1.38
17	P	5128	CLA	C2D-C1D	22.99	1.41	1.38
17	8	1013	CLA	C2D-C1D	22.98	1.41	1.38
17	F	4003	CLA	C2D-C1D	22.98	1.41	1.38
17	3	1032	CLA	C2D-C1D	22.98	1.41	1.38
17	G	1701	CLA	C2D-C1D	22.96	1.41	1.38
17	P	8009	CLA	C2D-C1D	22.95	1.41	1.38
17	0	1014	CLA	C2D-C1D	22.95	1.41	1.38
17	0	1012	CLA	C2D-C1D	22.95	1.41	1.38
17	P	5119	CLA	C2D-C1D	22.94	1.41	1.38
17	U	8006	CLA	C2D-C1D	22.93	1.41	1.38
17	Q	5228	CLA	C3D-C4D	22.93	1.41	1.38
17	4	1031	CLA	C2D-C1D	22.93	1.41	1.38
17	1	1031	CLA	C2D-C1D	22.92	1.41	1.38
17	4	1017	CLA	C2D-C1D	22.90	1.41	1.38
17	9	1012	CLA	C2D-C1D	22.89	1.41	1.38
17	8	1012	CLA	C2D-C1D	22.88	1.41	1.38
17	3	1022	CLA	C2D-C1D	22.86	1.41	1.38
17	A	4009	CLA	C2D-C1D	22.86	1.41	1.38
17	3	1012	CLA	C2D-C1D	22.85	1.41	1.38
17	0	1025	CLA	C2D-C1D	22.84	1.41	1.38
17	7	1031	CLA	C2D-C1D	22.84	1.41	1.38
17	Q	5217	CLA	C2D-C1D	22.83	1.41	1.38
17	A	1012	CLA	C2D-C1D	22.83	1.41	1.38
17	0	1031	CLA	C2D-C1D	22.83	1.41	1.38
17	Q	5237	CLA	C2A-C1A	22.81	1.50	1.39
17	B	1237	CLA	C2A-C1A	22.80	1.50	1.39
17	B	1214	CLA	C2D-C1D	22.78	1.41	1.38
17	0	1033	CLA	C2D-C1D	22.78	1.41	1.38
17	4	1014	CLA	C2D-C1D	22.77	1.41	1.38
17	9	1041	CLA	C2D-C1D	22.77	1.41	1.38
17	2	1012	CLA	C2D-C1D	22.76	1.41	1.38
17	2	1013	CLA	C2D-C1D	22.74	1.41	1.38
17	B	1228	CLA	C3D-C4D	22.74	1.41	1.38
17	8	1017	CLA	C2D-C1D	22.74	1.41	1.38
17	9	1022	CLA	C2D-C1D	22.72	1.41	1.38
17	Q	5214	CLA	C2D-C1D	22.70	1.41	1.38
17	2	1021	CLA	C2D-C1D	22.69	1.41	1.38
17	1	1015	CLA	C2D-C1D	22.68	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5012	CLA	C2D-C1D	22.65	1.41	1.38
17	9	1032	CLA	C2D-C1D	22.63	1.41	1.38
17	B	1217	CLA	C2D-C1D	22.59	1.41	1.38
17	9	1014	CLA	C2D-C1D	22.57	1.41	1.38
17	A	1128	CLA	C2D-C1D	22.56	1.41	1.38
17	1	1026	CLA	C2D-C1D	22.54	1.41	1.38
17	7	1015	CLA	C2D-C1D	22.54	1.41	1.38
17	V	5701	CLA	C2D-C1D	22.50	1.41	1.38
17	B	1241	CLA	C2D-C1D	22.46	1.41	1.38
17	8	1021	CLA	C2D-C1D	22.40	1.41	1.38
17	7	1026	CLA	C2D-C1D	22.33	1.41	1.38
17	3	1014	CLA	C2D-C1D	22.32	1.41	1.38
17	7	1011	CLA	C2D-C1D	22.31	1.41	1.38
17	B	1216	CLA	C2D-C1D	22.15	1.41	1.38
17	Q	5241	CLA	C2D-C1D	22.07	1.41	1.38
17	B	1222	CLA	C2D-C1D	22.06	1.41	1.38
17	P	5402	CLA	C2D-C1D	22.06	1.41	1.38
17	A	1110	CLA	C2D-C1D	22.04	1.41	1.38
17	P	5132	CLA	C2D-C1D	22.04	1.41	1.38
17	1	1011	CLA	C2D-C1D	21.99	1.41	1.38
17	P	5110	CLA	C2D-C1D	21.91	1.41	1.38
17	A	1402	CLA	C2D-C1D	21.90	1.41	1.38
17	2	4007	CLA	C2D-C1D	21.89	1.41	1.38
17	Q	5222	CLA	C2D-C1D	21.82	1.41	1.38
17	B	1204	CLA	C2D-C1D	21.82	1.41	1.38
17	A	1132	CLA	C2D-C1D	21.81	1.41	1.38
17	Q	5216	CLA	C2D-C1D	21.78	1.41	1.38
17	Q	5202	CLA	C2A-C1A	21.75	1.50	1.39
17	B	1202	CLA	C2A-C1A	21.72	1.50	1.39
17	8	8007	CLA	C2D-C1D	21.72	1.41	1.38
17	Q	5204	CLA	C2D-C1D	21.59	1.41	1.38
17	A	1133	CLA	C2D-C1D	21.58	1.41	1.38
17	P	5133	CLA	C2D-C1D	21.36	1.41	1.38
17	P	5139	CLA	C2D-C1D	21.24	1.41	1.38
17	B	1130	CLA	C2D-C1D	21.20	1.41	1.38
17	B	1232	CLA	C2D-C1D	21.08	1.41	1.38
17	A	1139	CLA	C2D-C1D	21.04	1.41	1.38
17	Q	5130	CLA	C2D-C1D	20.90	1.41	1.38
17	Q	5232	CLA	C2D-C1D	20.82	1.41	1.38
17	G	1233	CLA	C2D-C1D	20.73	1.41	1.38
17	V	5233	CLA	C2D-C1D	20.70	1.41	1.38
17	A	1011	CLA	C2D-C1D	20.67	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5011	CLA	C2D-C1D	20.60	1.41	1.38
17	6	5501	CLA	C3D-C4D	20.52	1.41	1.38
17	A	1104	CLA	C2D-C1D	20.52	1.41	1.38
17	P	5126	CLA	C3D-C4D	20.49	1.41	1.38
17	Q	5206	CLA	C2D-C1D	20.43	1.41	1.38
17	B	1206	CLA	C2D-C1D	20.42	1.41	1.38
17	B	1021	CLA	C2D-C1D	20.32	1.41	1.38
17	P	5102	CLA	C2D-C1D	20.23	1.41	1.38
17	Q	5021	CLA	C2D-C1D	20.23	1.41	1.38
17	L	1501	CLA	C3D-C4D	20.19	1.41	1.38
17	A	1126	CLA	C3D-C4D	20.12	1.41	1.38
17	A	1102	CLA	C2D-C1D	20.10	1.41	1.38
17	A	1901	CLA	C2D-C1D	19.95	1.41	1.38
17	A	1139	CLA	C3D-C4D	19.89	1.41	1.38
17	P	5104	CLA	C2D-C1D	19.89	1.41	1.38
17	B	1207	CLA	C3D-C4D	19.83	1.41	1.38
17	B	1210	CLA	C3D-C4D	19.80	1.41	1.38
17	Q	5210	CLA	C3D-C4D	19.75	1.41	1.38
17	P	5113	CLA	C3D-C4D	19.72	1.41	1.38
17	P	5901	CLA	C3D-C4D	19.66	1.41	1.38
17	B	1219	CLA	C3D-C4D	19.61	1.41	1.38
17	Q	5212	CLA	C2D-C1D	19.60	1.41	1.38
17	P	5139	CLA	C3D-C4D	19.58	1.41	1.38
17	Q	5219	CLA	C3D-C4D	19.55	1.41	1.38
17	B	1212	CLA	C2D-C1D	19.49	1.41	1.38
17	P	5901	CLA	C2D-C1D	19.48	1.41	1.38
17	A	1103	CLA	C3D-C4D	19.48	1.41	1.38
17	A	1901	CLA	C3D-C4D	19.43	1.41	1.38
17	A	1136	CLA	C3D-C4D	19.38	1.41	1.38
17	P	5136	CLA	C3D-C4D	19.38	1.41	1.38
17	P	5111	CLA	C3D-C4D	19.37	1.41	1.38
17	P	5103	CLA	C3D-C4D	19.37	1.41	1.38
17	Q	5207	CLA	C3D-C4D	19.35	1.41	1.38
19	C	3002	SF4	S1-FE2	-19.30	2.20	2.33
17	Q	5211	CLA	C3D-C4D	19.23	1.41	1.38
19	R	7002	SF4	S1-FE2	-19.22	2.20	2.33
17	A	1113	CLA	C3D-C4D	19.22	1.41	1.38
17	B	1211	CLA	C3D-C4D	19.13	1.41	1.38
17	A	1111	CLA	C3D-C4D	18.87	1.41	1.38
17	Q	5236	CLA	C2D-C1D	18.70	1.41	1.38
17	B	1236	CLA	C2D-C1D	18.45	1.41	1.38
17	P	5120	CLA	C3D-C4D	18.32	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1120	CLA	C3D-C4D	18.29	1.41	1.38
17	A	1109	CLA	C2D-C1D	18.19	1.41	1.38
17	F	1301	CLA	C3D-C4D	18.19	1.41	1.38
17	U	5301	CLA	C3D-C4D	18.11	1.41	1.38
17	P	5127	CLA	C3D-C4D	18.05	1.41	1.38
17	A	1105	CLA	C2D-C1D	17.97	1.41	1.38
17	A	1127	CLA	C3D-C4D	17.93	1.41	1.38
17	P	5109	CLA	C2D-C1D	17.90	1.41	1.38
17	P	5105	CLA	C2D-C1D	17.87	1.41	1.38
17	B	1218	CLA	C3D-C4D	17.56	1.41	1.38
17	A	1134	CLA	C3D-C4D	17.52	1.41	1.38
17	U	5301	CLA	C2D-C1D	17.49	1.41	1.38
17	B	1208	CLA	C3D-C4D	17.49	1.41	1.38
17	Q	5205	CLA	C3D-C4D	17.48	1.41	1.38
17	Q	5218	CLA	C3D-C4D	17.41	1.41	1.38
17	F	1301	CLA	C2D-C1D	17.41	1.41	1.38
17	B	1022	CLA	C2D-C1D	17.38	1.41	1.38
17	B	1205	CLA	C3D-C4D	17.38	1.41	1.38
17	Q	5208	CLA	C3D-C4D	17.31	1.41	1.38
17	P	5134	CLA	C3D-C4D	17.22	1.41	1.38
17	A	1013	CLA	C3D-C4D	17.09	1.41	1.38
19	C	3002	SF4	S4-FE3	-17.08	2.21	2.33
17	Q	5209	CLA	C3D-C4D	17.03	1.41	1.38
17	P	5128	CLA	C3D-C4D	17.03	1.41	1.38
19	R	7002	SF4	S4-FE3	-17.01	2.21	2.33
17	Q	5022	CLA	C2D-C1D	16.95	1.41	1.38
17	B	1209	CLA	C3D-C4D	16.83	1.41	1.38
17	B	1227	CLA	C3D-C4D	16.77	1.41	1.38
17	A	1128	CLA	C3D-C4D	16.77	1.41	1.38
17	V	5233	CLA	C3D-C4D	16.76	1.41	1.38
17	P	5112	CLA	C3D-C4D	16.74	1.41	1.38
17	B	1238	CLA	C3D-C4D	16.74	1.41	1.38
17	G	1233	CLA	C3D-C4D	16.70	1.41	1.38
17	A	1112	CLA	C3D-C4D	16.66	1.41	1.38
17	A	1131	CLA	C3D-C4D	16.63	1.41	1.38
17	A	1124	CLA	C3D-C4D	16.62	1.41	1.38
17	B	1207	CLA	C2D-C1D	16.61	1.41	1.38
17	P	5131	CLA	C3D-C4D	16.60	1.41	1.38
17	P	5124	CLA	C3D-C4D	16.56	1.41	1.38
17	Q	5227	CLA	C3D-C4D	16.54	1.41	1.38
17	P	5013	CLA	C3D-C4D	16.50	1.41	1.38
17	Q	5238	CLA	C3D-C4D	16.47	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1127	CLA	C2D-C1D	16.43	1.41	1.38
17	P	5127	CLA	C2D-C1D	16.35	1.41	1.38
17	B	1212	CLA	C3D-C4D	16.32	1.41	1.38
17	Q	5212	CLA	C3D-C4D	16.22	1.41	1.38
17	Q	5207	CLA	C2D-C1D	16.10	1.41	1.38
18	A	2001	PQN	O4-C4	16.09	1.42	1.22
18	P	6001	PQN	O4-C4	16.09	1.42	1.22
17	B	1226	CLA	C3D-C4D	16.06	1.41	1.38
17	A	1123	CLA	C3D-C4D	16.06	1.41	1.38
17	Q	5216	CLA	C3D-C4D	16.00	1.41	1.38
17	Q	5226	CLA	C3D-C4D	15.83	1.40	1.38
17	Q	5213	CLA	C3D-C4D	15.80	1.40	1.38
17	P	5123	CLA	C3D-C4D	15.78	1.40	1.38
17	B	1213	CLA	C3D-C4D	15.76	1.40	1.38
17	B	1216	CLA	C3D-C4D	15.76	1.40	1.38
17	Q	5232	CLA	C3D-C4D	15.65	1.40	1.38
18	Q	6002	PQN	O4-C4	15.57	1.42	1.22
18	B	2002	PQN	O4-C4	15.57	1.42	1.22
17	B	1232	CLA	C3D-C4D	15.50	1.40	1.38
17	B	1230	CLA	C3D-C4D	15.42	1.40	1.38
17	A	1138	CLA	C3D-C4D	15.42	1.40	1.38
17	Q	5230	CLA	C3D-C4D	15.36	1.40	1.38
17	A	1116	CLA	C2D-C1D	15.34	1.40	1.38
17	L	1503	CLA	C3D-C4D	15.33	1.40	1.38
17	P	5138	CLA	C3D-C4D	15.23	1.40	1.38
19	C	3002	SF4	S3-FE4	-15.14	2.23	2.33
17	B	1220	CLA	C3D-C4D	15.09	1.40	1.38
17	A	1106	CLA	C3D-C4D	15.02	1.40	1.38
19	R	7002	SF4	S3-FE4	-15.01	2.23	2.33
17	B	1237	CLA	C3D-C4D	15.00	1.40	1.38
17	P	5116	CLA	C2D-C1D	14.95	1.40	1.38
17	Q	5220	CLA	C3D-C4D	14.93	1.40	1.38
17	P	5107	CLA	C3D-C4D	14.80	1.40	1.38
17	6	5503	CLA	C3D-C4D	14.80	1.40	1.38
17	P	5106	CLA	C3D-C4D	14.78	1.40	1.38
17	Q	5237	CLA	C3D-C4D	14.76	1.40	1.38
17	B	1201	CLA	C3D-C4D	14.61	1.40	1.38
17	5	5401	CLA	C3D-C4D	14.57	1.40	1.38
17	A	1109	CLA	C3D-C4D	14.56	1.40	1.38
17	Q	5201	CLA	C3D-C4D	14.54	1.40	1.38
17	K	1401	CLA	C3D-C4D	14.40	1.40	1.38
17	P	5109	CLA	C3D-C4D	14.36	1.40	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1107	CLA	C3D-C4D	14.35	1.40	1.38
17	Q	5224	CLA	C3D-C4D	14.17	1.40	1.38
17	B	1217	CLA	C3D-C4D	14.13	1.40	1.38
17	Q	5231	CLA	C3D-C4D	14.11	1.40	1.38
17	B	1224	CLA	C3D-C4D	14.07	1.40	1.38
17	B	1231	CLA	C3D-C4D	14.06	1.40	1.38
17	Q	5217	CLA	C3D-C4D	14.06	1.40	1.38
17	8	1033	CLA	C3D-C4D	13.99	1.40	1.38
17	J	1302	CLA	C3D-C4D	13.98	1.40	1.38
19	R	7002	SF4	S2-FE1	-13.96	2.23	2.33
17	9	1016	CLA	C3D-C4D	13.95	1.40	1.38
17	4	1031	CLA	C3D-C4D	13.95	1.40	1.38
17	3	1016	CLA	C3D-C4D	13.93	1.40	1.38
17	0	1031	CLA	C3D-C4D	13.92	1.40	1.38
17	A	1114	CLA	C3D-C4D	13.89	1.40	1.38
17	9	1031	CLA	C3D-C4D	13.86	1.40	1.38
19	C	3002	SF4	S2-FE1	-13.86	2.23	2.33
17	B	1221	CLA	C3D-C4D	13.83	1.40	1.38
17	0	1017	CLA	C3D-C4D	13.76	1.40	1.38
17	0	1021	CLA	C3D-C4D	13.74	1.40	1.38
17	1	1015	CLA	C3D-C4D	13.74	1.40	1.38
17	B	1206	CLA	C3D-C4D	13.68	1.40	1.38
17	8	1011	CLA	C3D-C4D	13.68	1.40	1.38
17	P	5114	CLA	C3D-C4D	13.63	1.40	1.38
17	4	1017	CLA	C3D-C4D	13.60	1.40	1.38
17	Q	5221	CLA	C3D-C4D	13.60	1.40	1.38
17	4	1021	CLA	C3D-C4D	13.60	1.40	1.38
17	2	1023	CLA	C3D-C4D	13.60	1.40	1.38
17	2	1033	CLA	C3D-C4D	13.56	1.40	1.38
17	1	1025	CLA	C3D-C4D	13.53	1.40	1.38
17	7	1025	CLA	C3D-C4D	13.52	1.40	1.38
17	0	1014	CLA	C3D-C4D	13.50	1.40	1.38
17	Z	5302	CLA	C3D-C4D	13.49	1.40	1.38
17	4	1011	CLA	C3D-C4D	13.48	1.40	1.38
17	9	1032	CLA	C3D-C4D	13.47	1.40	1.38
17	0	1011	CLA	C3D-C4D	13.44	1.40	1.38
17	4	1023	CLA	C3D-C4D	13.44	1.40	1.38
17	3	1032	CLA	C3D-C4D	13.44	1.40	1.38
17	2	1021	CLA	C3D-C4D	13.43	1.40	1.38
17	9	1025	CLA	C3D-C4D	13.40	1.40	1.38
17	U	8006	CLA	C3D-C4D	13.39	1.40	1.38
17	2	1022	CLA	C3D-C4D	13.37	1.40	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	1032	CLA	C3D-C4D	13.37	1.40	1.38
17	3	1041	CLA	C3D-C4D	13.37	1.40	1.38
17	3	1017	CLA	C3D-C4D	13.36	1.40	1.38
17	0	1012	CLA	C3D-C4D	13.36	1.40	1.38
17	Q	5206	CLA	C3D-C4D	13.34	1.40	1.38
17	A	4009	CLA	C3D-C4D	13.33	1.40	1.38
17	A	1117	CLA	C3D-C4D	13.32	1.40	1.38
17	3	1012	CLA	C3D-C4D	13.31	1.40	1.38
17	7	1015	CLA	C3D-C4D	13.31	1.40	1.38
17	B	1240	CLA	C3D-C4D	13.31	1.40	1.38
17	9	1041	CLA	C3D-C4D	13.28	1.40	1.38
17	8	1023	CLA	C3D-C4D	13.28	1.40	1.38
17	0	1023	CLA	C3D-C4D	13.27	1.40	1.38
17	B	1204	CLA	C3D-C4D	13.25	1.40	1.38
17	A	4010	CLA	C3D-C4D	13.25	1.40	1.38
17	7	1016	CLA	C3D-C4D	13.25	1.40	1.38
17	8	1021	CLA	C3D-C4D	13.23	1.40	1.38
17	Q	5204	CLA	C3D-C4D	13.23	1.40	1.38
17	2	1025	CLA	C3D-C4D	13.23	1.40	1.38
17	0	1032	CLA	C3D-C4D	13.22	1.40	1.38
17	8	1022	CLA	C3D-C4D	13.20	1.40	1.38
17	9	1017	CLA	C3D-C4D	13.20	1.40	1.38
17	K	1404	CLA	C3D-C4D	13.20	1.40	1.38
17	4	1012	CLA	C3D-C4D	13.19	1.40	1.38
17	3	1031	CLA	C3D-C4D	13.17	1.40	1.38
17	P	5402	CLA	C3D-C4D	13.17	1.40	1.38
17	9	1022	CLA	C3D-C4D	13.17	1.40	1.38
17	7	1031	CLA	C3D-C4D	13.16	1.40	1.38
17	P	5118	CLA	C3D-C4D	13.15	1.40	1.38
17	9	1021	CLA	C3D-C4D	13.14	1.40	1.38
17	9	1012	CLA	C3D-C4D	13.14	1.40	1.38
17	F	4006	CLA	C3D-C4D	13.13	1.40	1.38
17	Z	5101	CLA	C3D-C4D	13.11	1.40	1.38
17	A	1118	CLA	C3D-C4D	13.11	1.40	1.38
17	9	1026	CLA	C3D-C4D	13.09	1.40	1.38
17	4	1014	CLA	C3D-C4D	13.07	1.40	1.38
17	Q	8001	CLA	C3D-C4D	13.06	1.40	1.38
17	F	4004	CLA	C3D-C4D	13.04	1.40	1.38
17	2	4007	CLA	C3D-C4D	13.03	1.40	1.38
17	Q	5214	CLA	C3D-C4D	13.02	1.40	1.38
17	8	1026	CLA	C3D-C4D	13.02	1.40	1.38
17	A	1402	CLA	C3D-C4D	13.02	1.40	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	0	1026	CLA	C3D-C4D	13.02	1.40	1.38
17	1	1013	CLA	C3D-C4D	13.02	1.40	1.38
17	J	4008	CLA	C3D-C4D	13.01	1.40	1.38
17	8	8007	CLA	C3D-C4D	13.01	1.40	1.38
17	0	1033	CLA	C3D-C4D	13.01	1.40	1.38
17	8	1025	CLA	C3D-C4D	13.00	1.40	1.38
17	G	1701	CLA	C3D-C4D	12.99	1.40	1.38
17	1	1016	CLA	C3D-C4D	12.99	1.40	1.38
17	7	1021	CLA	C3D-C4D	12.99	1.40	1.38
17	9	1033	CLA	C3D-C4D	12.98	1.40	1.38
17	4	1013	CLA	C3D-C4D	12.98	1.40	1.38
17	P	8010	CLA	C3D-C4D	12.97	1.40	1.38
17	U	8004	CLA	C3D-C4D	12.97	1.40	1.38
17	J	1101	CLA	C3D-C4D	12.97	1.40	1.38
17	P	5102	CLA	C3D-C4D	12.97	1.40	1.38
17	3	1021	CLA	C3D-C4D	12.97	1.40	1.38
17	P	5117	CLA	C3D-C4D	12.97	1.40	1.38
17	5	5403	CLA	C3D-C4D	12.94	1.40	1.38
17	4	1015	CLA	C3D-C4D	12.94	1.40	1.38
17	V	5701	CLA	C3D-C4D	12.94	1.40	1.38
17	3	1026	CLA	C3D-C4D	12.93	1.40	1.38
17	3	1022	CLA	C3D-C4D	12.93	1.40	1.38
17	7	1013	CLA	C3D-C4D	12.93	1.40	1.38
17	1	1031	CLA	C3D-C4D	12.92	1.40	1.38
17	7	1023	CLA	C3D-C4D	12.92	1.40	1.38
17	A	1133	CLA	C3D-C4D	12.90	1.40	1.38
17	Q	5240	CLA	C3D-C4D	12.90	1.40	1.38
17	8	1015	CLA	C3D-C4D	12.89	1.40	1.38
17	F	4003	CLA	C3D-C4D	12.89	1.40	1.38
17	W	5801	CLA	C3D-C4D	12.89	1.40	1.38
17	U	8003	CLA	C3D-C4D	12.88	1.40	1.38
17	3	1014	CLA	C3D-C4D	12.88	1.40	1.38
17	4	4002	CLA	C3D-C4D	12.88	1.40	1.38
17	Z	8008	CLA	C3D-C4D	12.88	1.40	1.38
17	P	8009	CLA	C3D-C4D	12.87	1.40	1.38
17	2	1011	CLA	C3D-C4D	12.87	1.40	1.38
17	B	1223	CLA	C3D-C4D	12.85	1.40	1.38
17	0	1016	CLA	C3D-C4D	12.83	1.40	1.38
17	L	1504	CLA	C3D-C4D	12.82	1.40	1.38
17	B	4001	CLA	C3D-C4D	12.82	1.40	1.38
17	4	1026	CLA	C3D-C4D	12.81	1.40	1.38
17	2	1026	CLA	C3D-C4D	12.81	1.40	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	1012	CLA	C3D-C4D	12.79	1.40	1.38
17	K	1403	CLA	C3D-C4D	12.78	1.40	1.38
17	4	1016	CLA	C3D-C4D	12.78	1.40	1.38
17	A	1102	CLA	C3D-C4D	12.76	1.40	1.38
17	1	1023	CLA	C3D-C4D	12.76	1.40	1.38
17	7	1017	CLA	C3D-C4D	12.75	1.40	1.38
17	3	1025	CLA	C3D-C4D	12.74	1.40	1.38
17	9	1014	CLA	C3D-C4D	12.73	1.40	1.38
17	9	1011	CLA	C3D-C4D	12.73	1.40	1.38
17	P	5133	CLA	C3D-C4D	12.72	1.40	1.38
17	4	1033	CLA	C3D-C4D	12.71	1.40	1.38
17	H	1801	CLA	C3D-C4D	12.71	1.40	1.38
17	2	1013	CLA	C3D-C4D	12.70	1.40	1.38
17	1	1021	CLA	C3D-C4D	12.68	1.40	1.38
17	Q	5242	CLA	C3D-C4D	12.68	1.40	1.38
17	6	5504	CLA	C3D-C4D	12.68	1.40	1.38
17	B	1214	CLA	C3D-C4D	12.68	1.40	1.38
17	Q	5223	CLA	C3D-C4D	12.67	1.40	1.38
17	0	1013	CLA	C3D-C4D	12.67	1.40	1.38
17	5	5404	CLA	C3D-C4D	12.66	1.40	1.38
17	B	1242	CLA	C3D-C4D	12.62	1.40	1.38
17	7	1011	CLA	C3D-C4D	12.61	1.40	1.38
17	2	1017	CLA	C3D-C4D	12.61	1.40	1.38
17	B	1222	CLA	C3D-C4D	12.60	1.40	1.38
17	0	8002	CLA	C3D-C4D	12.60	1.40	1.38
17	4	1025	CLA	C3D-C4D	12.60	1.40	1.38
17	2	1015	CLA	C3D-C4D	12.60	1.40	1.38
17	1	1017	CLA	C3D-C4D	12.56	1.40	1.38
17	3	1011	CLA	C3D-C4D	12.56	1.40	1.38
17	Q	5222	CLA	C3D-C4D	12.55	1.40	1.38
17	2	1031	CLA	C3D-C4D	12.55	1.40	1.38
17	2	1012	CLA	C3D-C4D	12.54	1.40	1.38
17	P	5125	CLA	C3D-C4D	12.53	1.40	1.38
17	4	1022	CLA	C3D-C4D	12.48	1.40	1.38
17	2	1016	CLA	C3D-C4D	12.48	1.40	1.38
17	0	1022	CLA	C3D-C4D	12.47	1.40	1.38
17	1	1026	CLA	C3D-C4D	12.47	1.40	1.38
17	0	1015	CLA	C3D-C4D	12.46	1.40	1.38
17	B	1239	CLA	C3D-C4D	12.45	1.40	1.38
17	1	1011	CLA	C3D-C4D	12.45	1.40	1.38
17	8	1012	CLA	C3D-C4D	12.44	1.40	1.38
17	3	1015	CLA	C3D-C4D	12.41	1.40	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	4005	CLA	C3D-C4D	12.41	1.40	1.38
17	8	1017	CLA	C3D-C4D	12.38	1.40	1.38
17	7	1012	CLA	C3D-C4D	12.36	1.40	1.38
17	3	1033	CLA	C3D-C4D	12.35	1.40	1.38
17	A	1125	CLA	C3D-C4D	12.33	1.40	1.38
17	0	1025	CLA	C3D-C4D	12.33	1.40	1.38
17	8	1016	CLA	C3D-C4D	12.30	1.40	1.38
17	8	1031	CLA	C3D-C4D	12.24	1.40	1.38
17	Q	5234	CLA	C3D-C4D	12.24	1.40	1.38
17	7	1026	CLA	C3D-C4D	12.19	1.40	1.38
17	Q	5239	CLA	C3D-C4D	12.17	1.40	1.38
17	8	1014	CLA	C3D-C4D	12.16	1.40	1.38
17	2	1014	CLA	C3D-C4D	12.16	1.40	1.38
17	P	5129	CLA	C3D-C4D	12.15	1.40	1.38
17	8	1013	CLA	C3D-C4D	12.13	1.40	1.38
17	1	1022	CLA	C3D-C4D	12.13	1.40	1.38
17	1	1014	CLA	C3D-C4D	12.12	1.40	1.38
17	B	1225	CLA	C3D-C4D	12.06	1.40	1.38
19	A	3001	SF4	S2-FE3	-11.88	2.25	2.33
17	Q	5225	CLA	C3D-C4D	11.88	1.40	1.38
19	P	7001	SF4	S2-FE3	-11.87	2.25	2.33
17	B	1234	CLA	C3D-C4D	11.85	1.40	1.38
17	7	1014	CLA	C3D-C4D	11.80	1.40	1.38
17	9	1015	CLA	C3D-C4D	11.76	1.40	1.38
17	U	8005	CLA	C3D-C4D	11.76	1.40	1.38
17	A	1129	CLA	C3D-C4D	11.73	1.40	1.38
17	U	5229	CLA	C3D-C4D	11.67	1.40	1.38
17	7	1022	CLA	C3D-C4D	11.58	1.40	1.38
17	F	1229	CLA	C3D-C4D	11.53	1.40	1.38
17	B	1241	CLA	C3D-C4D	11.43	1.40	1.38
17	P	5012	CLA	C3D-C4D	11.23	1.40	1.38
17	Q	5241	CLA	C3D-C4D	11.17	1.40	1.38
17	A	1115	CLA	C3D-C4D	10.98	1.40	1.38
17	A	1012	CLA	C3D-C4D	10.94	1.40	1.38
19	P	7001	SF4	S4-FE1	-10.92	2.25	2.33
17	Q	5203	CLA	C3D-C4D	10.91	1.40	1.38
17	P	5115	CLA	C3D-C4D	10.88	1.40	1.38
17	B	1203	CLA	C3D-C4D	10.86	1.40	1.38
17	Q	5130	CLA	C3D-C4D	10.84	1.40	1.38
17	Q	5215	CLA	C3D-C4D	10.84	1.40	1.38
19	A	3001	SF4	S4-FE1	-10.84	2.26	2.33
17	P	5104	CLA	C3D-C4D	10.77	1.40	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1215	CLA	C3D-C4D	10.74	1.40	1.38
17	A	1132	CLA	C3D-C4D	10.72	1.40	1.38
17	A	1104	CLA	C3D-C4D	10.70	1.40	1.38
17	B	1130	CLA	C3D-C4D	10.67	1.40	1.38
17	P	5132	CLA	C3D-C4D	10.51	1.40	1.38
17	P	5122	CLA	C3D-C4D	10.50	1.40	1.38
17	A	1122	CLA	C3D-C4D	10.45	1.40	1.38
17	A	1105	CLA	C3D-C4D	10.28	1.40	1.38
17	P	5108	CLA	C3D-C4D	10.20	1.40	1.38
17	A	1108	CLA	C3D-C4D	10.17	1.40	1.38
17	P	5105	CLA	C3D-C4D	10.15	1.40	1.38
17	Q	5202	CLA	C3D-C4D	10.08	1.40	1.38
17	A	1140	CLA	C3D-C4D	9.85	1.40	1.38
17	B	1202	CLA	C3D-C4D	9.78	1.40	1.38
17	Q	5235	CLA	C3D-C4D	9.76	1.40	1.38
17	P	5140	CLA	C3D-C4D	9.76	1.40	1.38
18	A	2001	PQN	C2M-C2	-9.65	1.36	1.51
18	P	6001	PQN	C2M-C2	-9.64	1.36	1.51
17	Q	5223	CLA	C2D-C1D	9.53	1.40	1.38
19	C	3003	SF4	S1-FE4	-9.52	2.26	2.33
19	A	3001	SF4	S1-FE4	-9.51	2.26	2.33
19	P	7001	SF4	S1-FE4	-9.49	2.26	2.33
19	R	7003	SF4	S1-FE4	-9.48	2.26	2.33
17	B	1235	CLA	C3D-C4D	9.47	1.40	1.38
18	Q	6002	PQN	C2M-C2	-9.28	1.37	1.51
18	B	2002	PQN	C2M-C2	-9.28	1.37	1.51
17	B	1223	CLA	C2D-C1D	9.16	1.40	1.38
19	A	3001	SF4	S1-FE2	-9.02	2.27	2.33
19	P	7001	SF4	S1-FE2	-9.01	2.27	2.33
18	A	2001	PQN	O1-C1	8.56	1.42	1.23
19	R	7003	SF4	S3-FE2	-8.56	2.27	2.33
19	C	3003	SF4	S3-FE2	-8.55	2.27	2.33
18	P	6001	PQN	O1-C1	8.53	1.42	1.23
17	P	5103	CLA	C4A-NA	-8.41	1.32	1.38
17	A	1103	CLA	C4A-NA	-8.40	1.32	1.38
17	P	5137	CLA	C3D-C4D	8.40	1.39	1.38
19	P	7001	SF4	S3-FE2	-8.34	2.27	2.33
17	A	1137	CLA	C3D-C4D	8.30	1.39	1.38
19	A	3001	SF4	S3-FE2	-8.19	2.27	2.33
18	Q	6002	PQN	O1-C1	8.13	1.41	1.23
18	B	2002	PQN	O1-C1	8.10	1.41	1.23
17	B	1202	CLA	C4A-NA	-8.03	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5202	CLA	C4A-NA	-8.03	1.32	1.38
19	P	7001	SF4	S2-FE4	-7.81	2.28	2.33
19	A	3001	SF4	S2-FE4	-7.72	2.28	2.33
17	A	1121	CLA	C3D-C4D	7.69	1.39	1.38
17	P	5121	CLA	C3D-C4D	7.69	1.39	1.38
17	Q	5203	CLA	C4A-NA	-7.56	1.32	1.38
17	B	1210	CLA	C4A-NA	-7.46	1.32	1.38
17	U	8003	CLA	C4A-NA	-7.43	1.32	1.38
17	Q	5022	CLA	C4A-NA	-7.43	1.32	1.38
17	B	1203	CLA	C4A-NA	-7.43	1.32	1.38
17	B	1022	CLA	C4A-NA	-7.42	1.32	1.38
17	0	1022	CLA	C4A-NA	-7.40	1.32	1.38
17	9	1014	CLA	C4A-NA	-7.39	1.32	1.38
17	3	1015	CLA	C4A-NA	-7.38	1.32	1.38
17	7	1011	CLA	C4A-NA	-7.38	1.32	1.38
17	Q	5210	CLA	C4A-NA	-7.37	1.32	1.38
17	9	1015	CLA	C4A-NA	-7.37	1.32	1.38
17	9	1033	CLA	C4A-NA	-7.36	1.32	1.38
17	5	5403	CLA	C4A-NA	-7.36	1.32	1.38
17	F	4003	CLA	C4A-NA	-7.35	1.32	1.38
17	P	5116	CLA	C3D-C4D	7.35	1.39	1.38
17	1	1011	CLA	C4A-NA	-7.34	1.32	1.38
17	4	1022	CLA	C4A-NA	-7.34	1.32	1.38
17	0	1031	CLA	C4A-NA	-7.34	1.32	1.38
17	P	8010	CLA	C4A-NA	-7.33	1.32	1.38
17	8	1021	CLA	C4A-NA	-7.33	1.32	1.38
17	3	1014	CLA	C4A-NA	-7.32	1.32	1.38
17	0	1033	CLA	C4A-NA	-7.31	1.32	1.38
17	7	1025	CLA	C4A-NA	-7.31	1.32	1.38
17	1	1013	CLA	C4A-NA	-7.31	1.32	1.38
17	8	1025	CLA	C4A-NA	-7.31	1.32	1.38
17	8	1016	CLA	C4A-NA	-7.30	1.32	1.38
17	3	1033	CLA	C4A-NA	-7.30	1.32	1.38
17	5	5404	CLA	C4A-NA	-7.29	1.32	1.38
17	2	1025	CLA	C4A-NA	-7.29	1.32	1.38
17	1	1025	CLA	C4A-NA	-7.29	1.32	1.38
17	2	1016	CLA	C4A-NA	-7.28	1.32	1.38
17	Q	8001	CLA	C4A-NA	-7.28	1.32	1.38
17	8	8007	CLA	C4A-NA	-7.28	1.32	1.38
17	1	1031	CLA	C4A-NA	-7.28	1.32	1.38
17	0	1015	CLA	C4A-NA	-7.28	1.32	1.38
17	4	1031	CLA	C4A-NA	-7.28	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	4010	CLA	C4A-NA	-7.28	1.32	1.38
17	7	1013	CLA	C4A-NA	-7.28	1.32	1.38
17	U	8004	CLA	C4A-NA	-7.27	1.32	1.38
17	3	1032	CLA	C4A-NA	-7.27	1.32	1.38
17	A	4009	CLA	C4A-NA	-7.27	1.32	1.38
17	4	1021	CLA	C4A-NA	-7.27	1.32	1.38
17	0	1021	CLA	C4A-NA	-7.26	1.32	1.38
17	9	1031	CLA	C4A-NA	-7.26	1.32	1.38
17	Z	5101	CLA	C4A-NA	-7.26	1.32	1.38
17	0	8002	CLA	C4A-NA	-7.26	1.32	1.38
17	2	1012	CLA	C4A-NA	-7.26	1.32	1.38
17	7	1017	CLA	C4A-NA	-7.26	1.32	1.38
17	8	1012	CLA	C4A-NA	-7.26	1.32	1.38
17	K	1404	CLA	C4A-NA	-7.26	1.32	1.38
17	8	1026	CLA	C4A-NA	-7.26	1.32	1.38
17	0	1013	CLA	C4A-NA	-7.26	1.32	1.38
17	F	4004	CLA	C4A-NA	-7.26	1.32	1.38
17	4	1033	CLA	C4A-NA	-7.26	1.32	1.38
17	9	1026	CLA	C4A-NA	-7.25	1.32	1.38
17	9	1032	CLA	C4A-NA	-7.25	1.33	1.38
17	2	4007	CLA	C4A-NA	-7.25	1.33	1.38
17	B	1242	CLA	C4A-NA	-7.25	1.33	1.38
17	3	1026	CLA	C4A-NA	-7.25	1.33	1.38
17	4	1013	CLA	C4A-NA	-7.25	1.33	1.38
17	Q	5240	CLA	C4A-NA	-7.25	1.33	1.38
17	0	1017	CLA	C4A-NA	-7.24	1.33	1.38
17	2	1021	CLA	C4A-NA	-7.24	1.33	1.38
17	4	1017	CLA	C4A-NA	-7.24	1.33	1.38
17	P	8009	CLA	C4A-NA	-7.24	1.33	1.38
17	3	1031	CLA	C4A-NA	-7.24	1.33	1.38
17	1	1017	CLA	C4A-NA	-7.24	1.33	1.38
17	Q	5242	CLA	C4A-NA	-7.24	1.33	1.38
17	G	1701	CLA	C4A-NA	-7.23	1.33	1.38
17	9	1011	CLA	C4A-NA	-7.23	1.33	1.38
17	9	1021	CLA	C4A-NA	-7.22	1.33	1.38
17	K	1403	CLA	C4A-NA	-7.22	1.33	1.38
17	7	1015	CLA	C4A-NA	-7.22	1.33	1.38
17	1	1021	CLA	C4A-NA	-7.22	1.33	1.38
17	7	1014	CLA	C4A-NA	-7.22	1.33	1.38
17	Q	5241	CLA	C4A-NA	-7.22	1.33	1.38
17	B	1240	CLA	C4A-NA	-7.22	1.33	1.38
17	4	4002	CLA	C4A-NA	-7.21	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	1025	CLA	C4A-NA	-7.21	1.33	1.38
17	2	1026	CLA	C4A-NA	-7.21	1.33	1.38
17	4	1015	CLA	C4A-NA	-7.21	1.33	1.38
17	J	4008	CLA	C4A-NA	-7.21	1.33	1.38
17	7	1022	CLA	C4A-NA	-7.21	1.33	1.38
17	2	1031	CLA	C4A-NA	-7.20	1.33	1.38
17	8	1011	CLA	C4A-NA	-7.20	1.33	1.38
17	W	5801	CLA	C4A-NA	-7.20	1.33	1.38
17	B	4001	CLA	C4A-NA	-7.20	1.33	1.38
17	8	1022	CLA	C4A-NA	-7.20	1.33	1.38
17	B	1241	CLA	C4A-NA	-7.20	1.33	1.38
17	2	1022	CLA	C4A-NA	-7.20	1.33	1.38
17	2	1014	CLA	C4A-NA	-7.20	1.33	1.38
17	1	1022	CLA	C4A-NA	-7.20	1.33	1.38
17	H	1801	CLA	C4A-NA	-7.19	1.33	1.38
17	7	1031	CLA	C4A-NA	-7.19	1.33	1.38
17	1	1014	CLA	C4A-NA	-7.19	1.33	1.38
17	J	1101	CLA	C4A-NA	-7.19	1.33	1.38
17	0	1026	CLA	C4A-NA	-7.19	1.33	1.38
17	1	1015	CLA	C4A-NA	-7.18	1.33	1.38
17	3	1021	CLA	C4A-NA	-7.18	1.33	1.38
17	9	1022	CLA	C4A-NA	-7.18	1.33	1.38
17	4	1014	CLA	C4A-NA	-7.17	1.33	1.38
17	2	1023	CLA	C4A-NA	-7.17	1.33	1.38
17	6	5502	CLA	C3D-C4D	7.17	1.39	1.38
17	3	1041	CLA	C4A-NA	-7.17	1.33	1.38
17	1	1023	CLA	C4A-NA	-7.17	1.33	1.38
17	3	1011	CLA	C4A-NA	-7.17	1.33	1.38
17	4	1011	CLA	C4A-NA	-7.17	1.33	1.38
17	3	1012	CLA	C4A-NA	-7.17	1.33	1.38
17	2	1011	CLA	C4A-NA	-7.17	1.33	1.38
17	4	1026	CLA	C4A-NA	-7.17	1.33	1.38
17	3	1022	CLA	C4A-NA	-7.17	1.33	1.38
17	4	1012	CLA	C4A-NA	-7.16	1.33	1.38
17	9	1017	CLA	C4A-NA	-7.16	1.33	1.38
17	V	5701	CLA	C4A-NA	-7.15	1.33	1.38
17	8	1014	CLA	C4A-NA	-7.15	1.33	1.38
17	8	1023	CLA	C4A-NA	-7.15	1.33	1.38
17	3	1017	CLA	C4A-NA	-7.15	1.33	1.38
17	4	1016	CLA	C4A-NA	-7.15	1.33	1.38
17	1	1016	CLA	C4A-NA	-7.15	1.33	1.38
17	4	1023	CLA	C4A-NA	-7.14	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	0	1025	CLA	C4A-NA	-7.14	1.33	1.38
17	Z	8008	CLA	C4A-NA	-7.14	1.33	1.38
17	2	1033	CLA	C4A-NA	-7.14	1.33	1.38
17	3	1025	CLA	C4A-NA	-7.13	1.33	1.38
17	7	1021	CLA	C4A-NA	-7.13	1.33	1.38
17	0	1014	CLA	C4A-NA	-7.13	1.33	1.38
17	4	1025	CLA	C4A-NA	-7.13	1.33	1.38
17	7	1023	CLA	C4A-NA	-7.13	1.33	1.38
17	8	1013	CLA	C4A-NA	-7.12	1.33	1.38
17	4	1032	CLA	C4A-NA	-7.12	1.33	1.38
17	0	1032	CLA	C4A-NA	-7.12	1.33	1.38
17	F	4006	CLA	C4A-NA	-7.12	1.33	1.38
17	0	1011	CLA	C4A-NA	-7.11	1.33	1.38
19	C	3002	SF4	S2-FE4	-7.11	2.28	2.33
17	8	1031	CLA	C4A-NA	-7.10	1.33	1.38
17	0	1023	CLA	C4A-NA	-7.10	1.33	1.38
17	8	1015	CLA	C4A-NA	-7.10	1.33	1.38
17	1	1026	CLA	C4A-NA	-7.09	1.33	1.38
17	7	1026	CLA	C4A-NA	-7.09	1.33	1.38
17	9	1041	CLA	C4A-NA	-7.09	1.33	1.38
17	9	1012	CLA	C4A-NA	-7.09	1.33	1.38
17	8	1017	CLA	C4A-NA	-7.09	1.33	1.38
17	6	5504	CLA	C4A-NA	-7.08	1.33	1.38
17	2	1015	CLA	C4A-NA	-7.08	1.33	1.38
17	7	1012	CLA	C4A-NA	-7.08	1.33	1.38
17	8	1033	CLA	C4A-NA	-7.08	1.33	1.38
17	1	1012	CLA	C4A-NA	-7.08	1.33	1.38
17	3	1016	CLA	C4A-NA	-7.07	1.33	1.38
17	9	1016	CLA	C4A-NA	-7.07	1.33	1.38
17	L	1504	CLA	C4A-NA	-7.07	1.33	1.38
17	7	1016	CLA	C4A-NA	-7.07	1.33	1.38
17	0	1012	CLA	C4A-NA	-7.07	1.33	1.38
17	0	1016	CLA	C4A-NA	-7.06	1.33	1.38
17	2	1013	CLA	C4A-NA	-7.05	1.33	1.38
17	U	8005	CLA	C4A-NA	-7.05	1.33	1.38
17	2	1017	CLA	C4A-NA	-7.04	1.33	1.38
19	R	7002	SF4	S2-FE4	-7.03	2.28	2.33
17	A	1012	CLA	C4A-NA	-7.02	1.33	1.38
17	U	8006	CLA	C4A-NA	-7.02	1.33	1.38
17	F	4005	CLA	C4A-NA	-7.01	1.33	1.38
17	P	5012	CLA	C4A-NA	-7.00	1.33	1.38
17	A	1116	CLA	C3D-C4D	6.95	1.39	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	3001	SF4	S1-FE3	-6.94	2.28	2.33
17	Q	5221	CLA	C4A-NA	-6.88	1.33	1.38
17	B	1221	CLA	C4A-NA	-6.87	1.33	1.38
19	P	7001	SF4	S1-FE3	-6.87	2.28	2.33
17	L	1502	CLA	C3D-C4D	6.80	1.39	1.38
17	1	1021	CLA	MG-NA	6.76	2.27	2.07
17	7	1021	CLA	MG-NA	6.73	2.27	2.07
17	P	5111	CLA	C4A-NA	-6.68	1.33	1.38
19	C	3003	SF4	S4-FE1	-6.67	2.28	2.33
19	R	7003	SF4	S4-FE1	-6.63	2.28	2.33
17	A	1111	CLA	C4A-NA	-6.61	1.33	1.38
17	A	1104	CLA	C4A-NA	-6.58	1.33	1.38
17	A	1901	CLA	C4A-NA	-6.58	1.33	1.38
19	A	3001	SF4	S2-FE1	-6.57	2.28	2.33
17	P	5104	CLA	C4A-NA	-6.57	1.33	1.38
19	P	7001	SF4	S2-FE1	-6.53	2.28	2.33
17	P	5901	CLA	C4A-NA	-6.51	1.33	1.38
19	C	3003	SF4	S2-FE4	-6.50	2.28	2.33
19	C	3002	SF4	S1-FE3	-6.49	2.28	2.33
19	R	7003	SF4	S2-FE4	-6.48	2.28	2.33
19	P	7001	SF4	S4-FE2	-6.45	2.28	2.33
19	R	7002	SF4	S1-FE3	-6.45	2.28	2.33
17	A	1125	CLA	C4A-NA	-6.44	1.33	1.38
17	P	5119	CLA	C3D-C4D	6.42	1.39	1.38
17	P	5125	CLA	C4A-NA	-6.40	1.33	1.38
17	A	1119	CLA	C3D-C4D	6.39	1.39	1.38
17	P	5402	CLA	C4A-NA	-6.39	1.33	1.38
19	R	7003	SF4	S1-FE2	-6.39	2.29	2.33
17	A	1132	CLA	C4A-NA	-6.37	1.33	1.38
19	A	3001	SF4	S4-FE2	-6.36	2.29	2.33
17	A	1402	CLA	C4A-NA	-6.36	1.33	1.38
17	P	5132	CLA	C4A-NA	-6.35	1.33	1.38
19	C	3003	SF4	S1-FE2	-6.34	2.29	2.33
17	B	1021	CLA	C4A-NA	-6.32	1.33	1.38
19	R	7003	SF4	S2-FE3	-6.29	2.29	2.33
17	Q	5021	CLA	C4A-NA	-6.29	1.33	1.38
19	C	3003	SF4	S2-FE3	-6.26	2.29	2.33
19	C	3002	SF4	S4-FE2	-6.26	2.29	2.33
19	R	7002	SF4	S4-FE2	-6.22	2.29	2.33
17	B	1234	CLA	C4A-NA	-6.20	1.33	1.38
17	Q	5236	CLA	C4A-NA	-6.16	1.33	1.38
17	A	1129	CLA	C4A-NA	-6.15	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1236	CLA	C4A-NA	-6.14	1.33	1.38
17	U	5229	CLA	C4A-NA	-6.13	1.33	1.38
17	J	1302	CLA	C4A-NA	-6.12	1.33	1.38
17	F	1229	CLA	C4A-NA	-6.11	1.33	1.38
17	Q	5234	CLA	C4A-NA	-6.11	1.33	1.38
17	P	5135	CLA	C4A-NA	-6.09	1.33	1.38
17	A	1135	CLA	C4A-NA	-6.05	1.33	1.38
17	P	5129	CLA	C4A-NA	-6.04	1.33	1.38
17	Z	5302	CLA	C4A-NA	-6.03	1.33	1.38
17	B	1236	CLA	C3D-C4D	5.97	1.39	1.38
17	Q	5236	CLA	C3D-C4D	5.96	1.39	1.38
17	Q	5219	CLA	C4A-NA	-5.90	1.33	1.38
17	B	1219	CLA	C4A-NA	-5.90	1.33	1.38
17	7	1021	CLA	MG-NB	5.88	2.18	2.05
17	Q	5022	CLA	C3D-C4D	5.87	1.39	1.38
17	1	1021	CLA	MG-NB	5.86	2.18	2.05
17	Q	5215	CLA	C4A-NA	-5.73	1.34	1.38
17	B	1022	CLA	C3D-C4D	5.72	1.39	1.38
17	Q	5206	CLA	C4A-NA	-5.70	1.34	1.38
17	B	1206	CLA	C4A-NA	-5.68	1.34	1.38
17	P	5127	CLA	C4A-NA	-5.67	1.34	1.38
17	P	5137	CLA	C4A-NA	-5.67	1.34	1.38
17	Q	5023	CLA	C4A-NA	-5.66	1.34	1.38
17	B	1023	CLA	C4A-NA	-5.66	1.34	1.38
17	A	1137	CLA	MG-NA	5.65	2.24	2.07
17	P	5137	CLA	MG-NA	5.65	2.24	2.07
17	A	1123	CLA	C4A-NA	-5.65	1.34	1.38
17	P	5123	CLA	MG-NA	5.63	2.23	2.07
17	A	1123	CLA	MG-NA	5.62	2.23	2.07
17	A	1013	CLA	C4A-NA	-5.61	1.34	1.38
17	A	1137	CLA	C4A-NA	-5.60	1.34	1.38
17	A	1119	CLA	C4A-NA	-5.59	1.34	1.38
17	A	1127	CLA	C4A-NA	-5.58	1.34	1.38
17	B	1215	CLA	C4A-NA	-5.57	1.34	1.38
17	P	5123	CLA	C4A-NA	-5.57	1.34	1.38
17	P	5119	CLA	C4A-NA	-5.52	1.34	1.38
17	Z	5302	CLA	MG-NA	5.51	2.23	2.07
17	Q	5224	CLA	C4A-NA	-5.50	1.34	1.38
17	Q	5204	CLA	C4A-NA	-5.50	1.34	1.38
17	B	1224	CLA	C4A-NA	-5.49	1.34	1.38
17	P	5013	CLA	C4A-NA	-5.49	1.34	1.38
17	J	1302	CLA	MG-NA	5.49	2.23	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1204	CLA	C4A-NA	-5.49	1.34	1.38
17	P	5011	CLA	C4A-NA	-5.45	1.34	1.38
17	A	1011	CLA	C4A-NA	-5.44	1.34	1.38
17	B	1221	CLA	MG-NA	5.43	2.23	2.07
17	Q	5221	CLA	MG-NA	5.43	2.23	2.07
17	A	1108	CLA	MG-NA	5.42	2.23	2.07
17	P	5108	CLA	MG-NA	5.41	2.23	2.07
17	Q	5210	CLA	MG-NA	5.36	2.23	2.07
17	B	1210	CLA	MG-NA	5.34	2.23	2.07
17	Q	5208	CLA	C4A-NA	-5.26	1.34	1.38
17	A	1126	CLA	C4A-NA	-5.22	1.34	1.38
17	B	1208	CLA	C4A-NA	-5.22	1.34	1.38
17	A	1901	CLA	MG-NA	5.22	2.22	2.07
17	P	5901	CLA	MG-NA	5.21	2.22	2.07
17	P	5012	CLA	MG-NA	5.19	2.22	2.07
17	A	1012	CLA	MG-NA	5.19	2.22	2.07
17	B	1231	CLA	C4A-NA	-5.17	1.34	1.38
17	P	5126	CLA	C4A-NA	-5.14	1.34	1.38
17	Q	5231	CLA	C4A-NA	-5.13	1.34	1.38
17	A	1108	CLA	C4A-NA	-5.13	1.34	1.38
17	Q	5207	CLA	MG-NA	5.10	2.22	2.07
17	P	5108	CLA	C4A-NA	-5.09	1.34	1.38
17	B	1207	CLA	MG-NA	5.08	2.22	2.07
17	6	5501	CLA	MG-NA	5.08	2.22	2.07
17	Q	5206	CLA	MG-NA	5.07	2.22	2.07
17	B	1206	CLA	MG-NA	5.06	2.22	2.07
17	L	1501	CLA	MG-NA	5.05	2.22	2.07
17	A	1113	CLA	MG-NA	5.03	2.22	2.07
17	P	5113	CLA	MG-NA	5.02	2.22	2.07
17	P	5402	CLA	MG-NA	4.99	2.22	2.07
17	A	1402	CLA	MG-NA	4.99	2.22	2.07
17	P	5131	CLA	MG-NA	4.96	2.21	2.07
17	A	1131	CLA	MG-NA	4.95	2.21	2.07
17	Q	5223	CLA	C4A-NA	-4.94	1.34	1.38
17	P	5108	CLA	MG-NB	4.94	2.16	2.05
17	B	1219	CLA	MG-NA	4.93	2.21	2.07
17	B	1223	CLA	C4A-NA	-4.93	1.34	1.38
17	Q	5219	CLA	MG-NA	4.93	2.21	2.07
17	B	1234	CLA	MG-NA	4.90	2.21	2.07
17	Q	5234	CLA	MG-NA	4.90	2.21	2.07
17	A	1108	CLA	MG-NB	4.90	2.15	2.05
17	P	5126	CLA	MG-NA	4.90	2.21	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1126	CLA	MG-NA	4.88	2.21	2.07
17	Q	5225	CLA	MG-NA	4.88	2.21	2.07
17	B	1225	CLA	MG-NA	4.85	2.21	2.07
17	B	1224	CLA	MG-NA	4.85	2.21	2.07
17	A	1112	CLA	MG-NA	4.84	2.21	2.07
17	Q	5224	CLA	MG-NA	4.84	2.21	2.07
17	J	1302	CLA	MG-NB	4.84	2.15	2.05
17	P	5112	CLA	MG-NA	4.83	2.21	2.07
17	Z	5302	CLA	MG-NB	4.82	2.15	2.05
17	P	5127	CLA	MG-NA	4.80	2.21	2.07
17	B	1232	CLA	MG-NA	4.79	2.21	2.07
17	A	1121	CLA	MG-NA	4.79	2.21	2.07
17	A	1127	CLA	MG-NA	4.79	2.21	2.07
17	A	1135	CLA	MG-NA	4.78	2.21	2.07
17	P	5135	CLA	MG-NA	4.78	2.21	2.07
17	Q	5232	CLA	MG-NA	4.78	2.21	2.07
17	B	1238	CLA	MG-NA	4.78	2.21	2.07
17	P	5121	CLA	MG-NA	4.77	2.21	2.07
17	B	1236	CLA	MG-NA	4.77	2.21	2.07
17	Q	5236	CLA	MG-NA	4.77	2.21	2.07
17	Q	5238	CLA	MG-NA	4.77	2.21	2.07
17	B	1213	CLA	MG-NA	4.72	2.21	2.07
17	P	5128	CLA	MG-NA	4.72	2.21	2.07
17	A	1115	CLA	MG-NA	4.71	2.21	2.07
17	Q	5213	CLA	MG-NA	4.71	2.21	2.07
17	Q	5228	CLA	C4A-NA	-4.71	1.34	1.38
17	Q	5220	CLA	MG-NA	4.70	2.21	2.07
17	Q	5225	CLA	C4A-NA	-4.70	1.34	1.38
17	B	1220	CLA	MG-NA	4.70	2.21	2.07
17	P	5115	CLA	MG-NA	4.70	2.21	2.07
17	A	1128	CLA	MG-NA	4.70	2.21	2.07
17	P	5124	CLA	C4A-NA	-4.68	1.34	1.38
17	P	5116	CLA	MG-NA	4.68	2.21	2.07
17	A	1116	CLA	MG-NA	4.68	2.21	2.07
17	A	1138	CLA	C4A-NA	-4.68	1.34	1.38
17	Q	5223	CLA	MG-NA	4.67	2.21	2.07
17	B	1225	CLA	C4A-NA	-4.66	1.34	1.38
17	B	1223	CLA	MG-NA	4.66	2.21	2.07
17	A	1133	CLA	C4A-NA	-4.66	1.34	1.38
17	A	1011	CLA	MG-NA	4.65	2.21	2.07
17	P	5138	CLA	C4A-NA	-4.65	1.34	1.38
17	P	5011	CLA	MG-NA	4.65	2.21	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1113	CLA	MG-NB	4.63	2.15	2.05
17	A	1124	CLA	C4A-NA	-4.63	1.34	1.38
17	P	5113	CLA	MG-NB	4.63	2.15	2.05
17	B	1228	CLA	C4A-NA	-4.62	1.34	1.38
17	Q	5237	CLA	C4A-NA	-4.61	1.34	1.38
17	Q	5202	CLA	MG-NA	4.61	2.20	2.07
17	A	1121	CLA	C4A-NA	-4.61	1.34	1.38
17	P	5133	CLA	C4A-NA	-4.61	1.34	1.38
17	B	1202	CLA	MG-NA	4.60	2.20	2.07
17	P	5105	CLA	MG-NA	4.60	2.20	2.07
17	P	5139	CLA	MG-NA	4.60	2.20	2.07
17	A	1139	CLA	MG-NA	4.60	2.20	2.07
17	B	1237	CLA	C4A-NA	-4.60	1.34	1.38
17	Q	5021	CLA	MG-NA	4.59	2.20	2.07
17	A	1105	CLA	MG-NA	4.59	2.20	2.07
17	B	1021	CLA	MG-NA	4.59	2.20	2.07
17	B	1203	CLA	MG-NA	4.58	2.20	2.07
17	Q	5203	CLA	MG-NA	4.57	2.20	2.07
17	A	1116	CLA	C4A-NA	-4.56	1.34	1.38
17	Q	5226	CLA	MG-NA	4.54	2.20	2.07
17	B	1232	CLA	C4A-NA	-4.54	1.34	1.38
19	R	7003	SF4	S2-FE1	-4.53	2.30	2.33
17	P	5102	CLA	MG-NA	4.53	2.20	2.07
17	A	1102	CLA	MG-NA	4.53	2.20	2.07
17	B	1210	CLA	MG-NB	4.52	2.15	2.05
17	B	1226	CLA	MG-NA	4.52	2.20	2.07
17	A	1104	CLA	MG-NA	4.52	2.20	2.07
17	P	5121	CLA	C4A-NA	-4.51	1.34	1.38
17	Q	5210	CLA	MG-NB	4.51	2.15	2.05
17	P	5116	CLA	C4A-NA	-4.50	1.34	1.38
17	A	1103	CLA	MG-NB	4.50	2.15	2.05
17	P	5104	CLA	MG-NA	4.49	2.20	2.07
17	7	1013	CLA	MG-NA	4.49	2.20	2.07
17	9	1011	CLA	MG-NA	4.49	2.20	2.07
17	6	5503	CLA	MG-NA	4.49	2.20	2.07
17	3	1025	CLA	MG-NA	4.48	2.20	2.07
17	7	1011	CLA	MG-NA	4.48	2.20	2.07
17	3	1011	CLA	MG-NA	4.48	2.20	2.07
17	0	1015	CLA	MG-NA	4.48	2.20	2.07
17	L	1503	CLA	MG-NA	4.48	2.20	2.07
17	Q	5212	CLA	MG-NA	4.48	2.20	2.07
17	3	1032	CLA	MG-NA	4.48	2.20	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	3003	SF4	S2-FE1	-4.48	2.30	2.33
17	P	5103	CLA	MG-NB	4.48	2.15	2.05
17	0	1032	CLA	MG-NA	4.47	2.20	2.07
17	B	1211	CLA	C4A-NA	-4.47	1.34	1.38
17	1	1013	CLA	MG-NA	4.48	2.20	2.07
17	2	1025	CLA	MG-NA	4.47	2.20	2.07
17	9	1032	CLA	MG-NA	4.47	2.20	2.07
17	1	1011	CLA	MG-NA	4.47	2.20	2.07
17	4	1032	CLA	MG-NA	4.47	2.20	2.07
17	8	1026	CLA	MG-NA	4.47	2.20	2.07
17	Q	5219	CLA	MG-NB	4.47	2.14	2.05
17	8	1033	CLA	MG-NA	4.47	2.20	2.07
17	Q	5203	CLA	MG-NB	4.47	2.14	2.05
17	8	1016	CLA	MG-NA	4.47	2.20	2.07
17	8	8007	CLA	MG-NA	4.47	2.20	2.07
17	0	8002	CLA	MG-NA	4.46	2.20	2.07
17	8	1025	CLA	MG-NA	4.46	2.20	2.07
17	9	1033	CLA	MG-NA	4.46	2.20	2.07
17	4	1015	CLA	MG-NA	4.46	2.20	2.07
17	B	1212	CLA	MG-NA	4.46	2.20	2.07
17	B	1219	CLA	MG-NB	4.47	2.14	2.05
17	9	1025	CLA	MG-NA	4.46	2.20	2.07
17	3	1022	CLA	MG-NA	4.46	2.20	2.07
17	0	1012	CLA	MG-NA	4.46	2.20	2.07
17	1	1031	CLA	MG-NA	4.46	2.20	2.07
17	K	1401	CLA	MG-NA	4.46	2.20	2.07
17	0	1031	CLA	MG-NA	4.46	2.20	2.07
17	2	1026	CLA	MG-NA	4.46	2.20	2.07
17	9	1031	CLA	MG-NA	4.46	2.20	2.07
17	Q	5232	CLA	C4A-NA	-4.46	1.34	1.38
17	2	1022	CLA	MG-NA	4.46	2.20	2.07
17	9	1022	CLA	MG-NA	4.46	2.20	2.07
17	9	1012	CLA	MG-NA	4.46	2.20	2.07
17	4	1012	CLA	MG-NA	4.46	2.20	2.07
17	8	1014	CLA	MG-NA	4.46	2.20	2.07
17	8	1022	CLA	MG-NA	4.46	2.20	2.07
17	Z	5101	CLA	MG-NA	4.46	2.20	2.07
17	2	1033	CLA	MG-NA	4.46	2.20	2.07
17	2	1016	CLA	MG-NA	4.46	2.20	2.07
17	9	1017	CLA	MG-NA	4.46	2.20	2.07
17	4	1031	CLA	MG-NA	4.46	2.20	2.07
17	4	4002	CLA	MG-NA	4.46	2.20	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	4007	CLA	MG-NA	4.45	2.20	2.07
17	B	1242	CLA	MG-NA	4.45	2.20	2.07
17	3	1015	CLA	MG-NA	4.45	2.20	2.07
17	5	5401	CLA	MG-NA	4.45	2.20	2.07
17	0	1011	CLA	MG-NA	4.45	2.20	2.07
17	8	1031	CLA	MG-NA	4.45	2.20	2.07
17	7	1031	CLA	MG-NA	4.45	2.20	2.07
17	1	1022	CLA	MG-NA	4.45	2.20	2.07
17	F	4006	CLA	MG-NA	4.45	2.20	2.07
17	3	1012	CLA	MG-NA	4.45	2.20	2.07
17	7	1015	CLA	MG-NA	4.45	2.20	2.07
17	6	5504	CLA	MG-NA	4.45	2.20	2.07
17	4	1011	CLA	MG-NA	4.45	2.20	2.07
17	W	5801	CLA	MG-NA	4.45	2.20	2.07
17	3	1033	CLA	MG-NA	4.45	2.20	2.07
17	3	1031	CLA	MG-NA	4.45	2.20	2.07
17	A	4009	CLA	MG-NA	4.45	2.20	2.07
17	1	1014	CLA	MG-NA	4.45	2.20	2.07
17	Q	5211	CLA	C4A-NA	-4.45	1.34	1.38
17	1	1026	CLA	MG-NA	4.45	2.20	2.07
17	U	8006	CLA	MG-NA	4.45	2.20	2.07
17	1	1015	CLA	MG-NA	4.45	2.20	2.07
17	B	1203	CLA	MG-NB	4.44	2.14	2.05
17	G	1701	CLA	MG-NA	4.44	2.20	2.07
17	5	5403	CLA	MG-NA	4.44	2.20	2.07
17	9	1015	CLA	MG-NA	4.44	2.20	2.07
17	4	1033	CLA	MG-NA	4.44	2.20	2.07
17	0	1023	CLA	MG-NA	4.44	2.20	2.07
17	2	1011	CLA	MG-NA	4.44	2.20	2.07
17	U	8005	CLA	MG-NA	4.44	2.20	2.07
17	V	5701	CLA	MG-NA	4.44	2.20	2.07
17	3	1017	CLA	MG-NA	4.44	2.20	2.07
17	0	1022	CLA	MG-NA	4.44	2.20	2.07
17	3	1021	CLA	MG-NA	4.44	2.20	2.07
17	4	1022	CLA	MG-NA	4.44	2.20	2.07
17	Q	5241	CLA	MG-NA	4.44	2.20	2.07
17	2	1017	CLA	MG-NA	4.44	2.20	2.07
17	1	1017	CLA	MG-NA	4.44	2.20	2.07
17	J	1101	CLA	MG-NA	4.44	2.20	2.07
17	7	1016	CLA	MG-NA	4.44	2.20	2.07
17	4	1023	CLA	MG-NA	4.44	2.20	2.07
17	3	1014	CLA	MG-NA	4.44	2.20	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	8009	CLA	MG-NA	4.44	2.20	2.07
17	U	8004	CLA	MG-NA	4.44	2.20	2.07
17	L	1504	CLA	MG-NA	4.44	2.20	2.07
17	2	1031	CLA	MG-NA	4.44	2.20	2.07
17	A	4010	CLA	MG-NA	4.44	2.20	2.07
17	1	1012	CLA	MG-NA	4.43	2.20	2.07
17	9	1026	CLA	MG-NA	4.43	2.20	2.07
17	9	1021	CLA	MG-NA	4.43	2.20	2.07
17	F	4005	CLA	MG-NA	4.43	2.20	2.07
17	Q	5240	CLA	MG-NA	4.43	2.20	2.07
17	5	5404	CLA	MG-NA	4.44	2.20	2.07
17	3	1026	CLA	MG-NA	4.43	2.20	2.07
17	J	4008	CLA	MG-NA	4.43	2.20	2.07
17	H	1801	CLA	MG-NA	4.43	2.20	2.07
17	K	1404	CLA	MG-NA	4.43	2.20	2.07
17	B	1240	CLA	MG-NA	4.43	2.20	2.07
17	K	1403	CLA	MG-NA	4.43	2.20	2.07
17	8	1013	CLA	MG-NA	4.43	2.20	2.07
17	2	1014	CLA	MG-NA	4.43	2.20	2.07
17	0	1026	CLA	MG-NA	4.43	2.20	2.07
17	F	4003	CLA	MG-NA	4.43	2.20	2.07
17	7	1022	CLA	MG-NA	4.43	2.20	2.07
17	9	1016	CLA	MG-NA	4.43	2.20	2.07
17	7	1017	CLA	MG-NA	4.43	2.20	2.07
17	P	8010	CLA	MG-NA	4.43	2.20	2.07
17	B	1241	CLA	MG-NA	4.43	2.20	2.07
17	8	1011	CLA	MG-NA	4.43	2.20	2.07
17	8	1012	CLA	MG-NA	4.43	2.20	2.07
17	F	4004	CLA	MG-NA	4.43	2.20	2.07
17	1	1023	CLA	MG-NA	4.43	2.20	2.07
17	7	1012	CLA	MG-NA	4.43	2.20	2.07
17	B	4001	CLA	MG-NA	4.43	2.20	2.07
17	Q	5242	CLA	MG-NA	4.43	2.20	2.07
17	1	1016	CLA	MG-NA	4.43	2.20	2.07
17	8	1021	CLA	MG-NA	4.43	2.20	2.07
17	4	1017	CLA	MG-NA	4.42	2.20	2.07
17	Q	8001	CLA	MG-NA	4.42	2.20	2.07
17	2	1012	CLA	MG-NA	4.42	2.20	2.07
17	7	1026	CLA	MG-NA	4.42	2.20	2.07
17	2	1013	CLA	MG-NA	4.42	2.20	2.07
17	7	1014	CLA	MG-NA	4.42	2.20	2.07
17	0	1033	CLA	MG-NA	4.42	2.20	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	1026	CLA	MG-NA	4.42	2.20	2.07
17	8	1017	CLA	MG-NA	4.42	2.20	2.07
17	B	1201	CLA	C4A-NA	-4.42	1.34	1.38
17	P	5114	CLA	MG-NA	4.42	2.20	2.07
17	3	1041	CLA	MG-NA	4.42	2.20	2.07
17	3	1016	CLA	MG-NA	4.41	2.20	2.07
17	Z	8008	CLA	MG-NA	4.41	2.20	2.07
17	U	8003	CLA	MG-NA	4.41	2.20	2.07
17	B	1202	CLA	MG-NB	4.41	2.14	2.05
17	2	1023	CLA	MG-NA	4.41	2.20	2.07
17	2	1021	CLA	MG-NA	4.41	2.20	2.07
17	1	1025	CLA	MG-NA	4.41	2.20	2.07
17	7	1023	CLA	MG-NA	4.41	2.20	2.07
17	Q	5202	CLA	MG-NB	4.41	2.14	2.05
17	9	1041	CLA	MG-NA	4.41	2.20	2.07
17	9	1014	CLA	MG-NA	4.41	2.20	2.07
17	A	1114	CLA	MG-NA	4.40	2.20	2.07
17	4	1014	CLA	MG-NA	4.40	2.20	2.07
17	4	1013	CLA	MG-NA	4.40	2.20	2.07
17	0	1014	CLA	MG-NA	4.40	2.20	2.07
17	2	1015	CLA	MG-NA	4.40	2.20	2.07
17	0	1017	CLA	MG-NA	4.39	2.20	2.07
17	0	1016	CLA	MG-NA	4.39	2.20	2.07
17	0	1021	CLA	MG-NA	4.39	2.20	2.07
17	7	1025	CLA	MG-NA	4.39	2.20	2.07
17	4	1021	CLA	MG-NA	4.39	2.20	2.07
17	Q	5201	CLA	C4A-NA	-4.39	1.34	1.38
17	0	1013	CLA	MG-NA	4.39	2.20	2.07
17	8	1015	CLA	MG-NA	4.38	2.20	2.07
17	8	1023	CLA	MG-NA	4.38	2.20	2.07
17	4	1016	CLA	MG-NA	4.38	2.20	2.07
17	4	1025	CLA	MG-NA	4.38	2.20	2.07
17	P	5128	CLA	MG-NB	4.37	2.14	2.05
17	0	1025	CLA	MG-NA	4.36	2.20	2.07
17	Q	5022	CLA	MG-NA	4.36	2.20	2.07
17	G	1233	CLA	MG-NA	4.36	2.20	2.07
17	B	1022	CLA	MG-NA	4.35	2.20	2.07
17	Q	5208	CLA	MG-NA	4.35	2.20	2.07
17	P	5117	CLA	MG-NA	4.35	2.20	2.07
19	P	7001	SF4	S4-FE3	-4.34	2.30	2.33
17	A	1117	CLA	MG-NA	4.35	2.20	2.07
17	V	5233	CLA	MG-NA	4.34	2.20	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	U	5301	CLA	MG-NA	4.34	2.20	2.07
17	A	1120	CLA	C4A-NA	-4.34	1.35	1.38
17	B	1208	CLA	MG-NA	4.34	2.20	2.07
17	B	1218	CLA	MG-NA	4.33	2.20	2.07
17	A	1128	CLA	MG-NB	4.33	2.14	2.05
17	F	1301	CLA	MG-NA	4.33	2.20	2.07
17	Q	5222	CLA	C4A-NA	-4.32	1.35	1.38
17	Q	5216	CLA	MG-NA	4.32	2.20	2.07
17	B	1216	CLA	MG-NA	4.32	2.20	2.07
17	B	1211	CLA	MG-NA	4.31	2.20	2.07
19	A	3001	SF4	S4-FE3	-4.31	2.30	2.33
17	Q	5218	CLA	MG-NA	4.31	2.20	2.07
17	Q	5211	CLA	MG-NA	4.31	2.20	2.07
17	B	1222	CLA	C4A-NA	-4.30	1.35	1.38
17	Q	5207	CLA	MG-NB	4.30	2.14	2.05
17	B	1207	CLA	MG-NB	4.29	2.14	2.05
17	B	1217	CLA	MG-NA	4.29	2.19	2.07
17	A	1125	CLA	MG-NA	4.29	2.19	2.07
19	C	3003	SF4	S4-FE2	-4.28	2.30	2.33
17	A	1118	CLA	C4A-NA	-4.28	1.35	1.38
17	Q	5214	CLA	C4A-NA	-4.28	1.35	1.38
17	P	5125	CLA	MG-NA	4.27	2.19	2.07
17	Q	5217	CLA	MG-NA	4.27	2.19	2.07
17	P	5120	CLA	C4A-NA	-4.26	1.35	1.38
17	P	5118	CLA	C4A-NA	-4.26	1.35	1.38
17	P	5106	CLA	C4A-NA	-4.25	1.35	1.38
17	A	1136	CLA	MG-NA	4.25	2.19	2.07
17	B	1214	CLA	C4A-NA	-4.25	1.35	1.38
17	P	5136	CLA	MG-NA	4.25	2.19	2.07
19	R	7003	SF4	S4-FE2	-4.24	2.30	2.33
17	Q	5215	CLA	MG-NA	4.23	2.19	2.07
17	Q	5227	CLA	C4A-NA	-4.22	1.35	1.38
17	B	1215	CLA	MG-NA	4.22	2.19	2.07
17	B	1230	CLA	C4A-NA	-4.21	1.35	1.38
17	P	5137	CLA	MG-NB	4.20	2.14	2.05
17	P	5134	CLA	MG-NA	4.20	2.19	2.07
17	P	5111	CLA	MG-NA	4.20	2.19	2.07
17	A	1134	CLA	MG-NA	4.19	2.19	2.07
17	Q	5226	CLA	C4A-NA	-4.19	1.35	1.38
17	A	1137	CLA	MG-NB	4.18	2.14	2.05
17	A	1111	CLA	MG-NA	4.18	2.19	2.07
17	B	1227	CLA	C4A-NA	-4.17	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5230	CLA	C4A-NA	-4.16	1.35	1.38
17	B	1226	CLA	C4A-NA	-4.15	1.35	1.38
17	A	1120	CLA	MG-NA	4.14	2.19	2.07
17	A	1106	CLA	C4A-NA	-4.14	1.35	1.38
17	Q	5209	CLA	MG-NA	4.14	2.19	2.07
17	A	1118	CLA	MG-NA	4.13	2.19	2.07
17	P	5120	CLA	MG-NA	4.13	2.19	2.07
17	B	1209	CLA	MG-NA	4.12	2.19	2.07
17	P	5134	CLA	C4A-NA	-4.12	1.35	1.38
17	P	5118	CLA	MG-NA	4.12	2.19	2.07
17	6	5503	CLA	C4A-NA	-4.12	1.35	1.38
17	A	1135	CLA	MG-NB	4.11	2.14	2.05
17	7	1021	CLA	MG-ND	-4.11	1.95	2.05
17	B	1223	CLA	MG-NB	4.10	2.14	2.05
17	1	1021	CLA	MG-ND	-4.10	1.95	2.05
17	A	1107	CLA	MG-NA	4.10	2.19	2.07
17	P	5107	CLA	MG-NA	4.09	2.19	2.07
17	P	5135	CLA	MG-NB	4.08	2.14	2.05
17	Q	5223	CLA	MG-NB	4.08	2.14	2.05
17	A	1117	CLA	C4A-NA	-4.08	1.35	1.38
17	Q	5201	CLA	MG-NA	4.08	2.19	2.07
17	B	1201	CLA	MG-NA	4.08	2.19	2.07
17	B	1205	CLA	MG-NA	4.08	2.19	2.07
19	C	3003	SF4	S3-FE4	-4.06	2.30	2.33
17	Q	5205	CLA	MG-NA	4.06	2.19	2.07
17	6	5502	CLA	MG-NA	4.05	2.19	2.07
17	L	1502	CLA	MG-NA	4.05	2.19	2.07
17	A	1122	CLA	MG-NA	4.05	2.19	2.07
17	P	5122	CLA	MG-NA	4.05	2.19	2.07
17	A	1134	CLA	C4A-NA	-4.05	1.35	1.38
17	B	1205	CLA	MG-NB	4.05	2.14	2.05
17	Q	5205	CLA	MG-NB	4.05	2.14	2.05
17	Q	5227	CLA	MG-NA	4.04	2.19	2.07
17	P	5402	CLA	MG-NB	4.03	2.14	2.05
17	A	1402	CLA	MG-NB	4.03	2.14	2.05
17	B	1227	CLA	MG-NA	4.03	2.19	2.07
17	P	5117	CLA	C4A-NA	-4.02	1.35	1.38
17	B	1222	CLA	MG-NA	4.01	2.19	2.07
17	L	1503	CLA	C4A-NA	-4.01	1.35	1.38
17	Q	5222	CLA	MG-NA	4.00	2.19	2.07
19	R	7003	SF4	S3-FE4	-4.00	2.30	2.33
17	P	5013	CLA	MG-NB	3.98	2.13	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1013	CLA	MG-NB	3.97	2.13	2.05
17	Q	5228	CLA	MG-NA	3.97	2.19	2.07
17	A	1119	CLA	MG-NA	3.97	2.19	2.07
17	P	5107	CLA	C4A-NA	-3.97	1.35	1.38
17	A	1131	CLA	C4A-NA	-3.96	1.35	1.38
19	P	7001	SF4	S3-FE1	-3.96	2.30	2.33
17	P	5119	CLA	MG-NA	3.96	2.18	2.07
19	A	3001	SF4	S3-FE1	-3.95	2.30	2.33
17	B	1228	CLA	MG-NA	3.95	2.18	2.07
17	P	5109	CLA	MG-NA	3.95	2.18	2.07
17	P	5131	CLA	C4A-NA	-3.95	1.35	1.38
17	P	5110	CLA	MG-NA	3.95	2.18	2.07
17	A	1110	CLA	MG-NA	3.94	2.18	2.07
17	A	1109	CLA	MG-NA	3.94	2.18	2.07
17	B	1221	CLA	MG-NB	3.92	2.13	2.05
17	A	1133	CLA	MG-NA	3.92	2.18	2.07
17	P	5106	CLA	MG-NA	3.92	2.18	2.07
17	P	5133	CLA	MG-NA	3.92	2.18	2.07
17	Q	5221	CLA	MG-NB	3.92	2.13	2.05
17	A	1013	CLA	MG-NA	3.91	2.18	2.07
18	Q	6002	PQN	C10-C5	3.91	1.46	1.40
17	A	1106	CLA	MG-NA	3.91	2.18	2.07
17	A	1107	CLA	C4A-NA	-3.91	1.35	1.38
17	A	1104	CLA	MG-NB	3.90	2.13	2.05
17	P	5013	CLA	MG-NA	3.90	2.18	2.07
17	P	5125	CLA	MG-NB	3.89	2.13	2.05
17	A	1125	CLA	MG-NB	3.89	2.13	2.05
17	B	1230	CLA	MG-NA	3.88	2.18	2.07
17	Q	5230	CLA	MG-NA	3.88	2.18	2.07
17	P	5104	CLA	MG-NB	3.87	2.13	2.05
18	B	2002	PQN	C10-C5	3.87	1.46	1.40
19	C	3003	SF4	S1-FE3	-3.86	2.30	2.33
17	B	1214	CLA	MG-NA	3.86	2.18	2.07
17	Q	5214	CLA	MG-NA	3.85	2.18	2.07
17	A	1112	CLA	C4A-NA	-3.84	1.35	1.38
17	U	5229	CLA	MG-NA	3.84	2.18	2.07
17	F	1229	CLA	MG-NA	3.83	2.18	2.07
17	Q	5023	CLA	MG-NA	3.83	2.18	2.07
17	A	1140	CLA	MG-NA	3.83	2.18	2.07
17	A	1901	CLA	MG-NB	3.82	2.13	2.05
17	P	5140	CLA	MG-NA	3.82	2.18	2.07
17	P	5901	CLA	MG-NB	3.82	2.13	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1023	CLA	MG-NA	3.81	2.18	2.07
17	B	1235	CLA	C4A-NA	-3.81	1.35	1.38
17	B	1231	CLA	MG-NA	3.80	2.18	2.07
19	P	7001	SF4	S3-FE4	-3.80	2.30	2.33
17	P	5112	CLA	C4A-NA	-3.80	1.35	1.38
17	A	1103	CLA	MG-NA	3.78	2.18	2.07
17	B	1212	CLA	C4A-NA	-3.78	1.35	1.38
17	Q	5212	CLA	C4A-NA	-3.78	1.35	1.38
17	Q	5231	CLA	MG-NA	3.77	2.18	2.07
17	P	5103	CLA	MG-NA	3.77	2.18	2.07
17	B	1130	CLA	C4A-NA	-3.77	1.35	1.38
19	A	3001	SF4	S3-FE4	-3.77	2.30	2.33
19	R	7003	SF4	S1-FE3	-3.76	2.30	2.33
17	P	5138	CLA	MG-NA	3.75	2.18	2.07
17	A	1138	CLA	MG-NA	3.75	2.18	2.07
17	Q	5235	CLA	C4A-NA	-3.74	1.35	1.38
17	A	1137	CLA	MG-NC	3.72	2.18	2.07
17	P	5137	CLA	MG-NC	3.72	2.18	2.07
17	Q	5130	CLA	C4A-NA	-3.71	1.35	1.38
17	Q	5207	CLA	C4A-NA	-3.71	1.35	1.38
17	B	1207	CLA	C4A-NA	-3.70	1.35	1.38
17	B	1022	CLA	MG-NB	3.70	2.13	2.05
17	Q	5022	CLA	MG-NB	3.70	2.13	2.05
17	Q	5234	CLA	MG-NB	3.69	2.13	2.05
17	P	5109	CLA	C4A-NA	-3.68	1.35	1.38
17	B	1234	CLA	MG-NB	3.68	2.13	2.05
17	A	1129	CLA	MG-NA	3.67	2.18	2.07
17	P	5115	CLA	MG-NB	3.67	2.13	2.05
17	A	1115	CLA	MG-NB	3.66	2.13	2.05
17	P	5129	CLA	MG-NA	3.66	2.18	2.07
17	A	1109	CLA	C4A-NA	-3.65	1.35	1.38
17	6	5502	CLA	MG-NB	3.63	2.13	2.05
17	P	5132	CLA	MG-NA	3.63	2.18	2.07
17	A	1136	CLA	MG-NB	3.62	2.13	2.05
17	P	5136	CLA	MG-NB	3.62	2.13	2.05
17	A	1132	CLA	MG-NA	3.62	2.17	2.07
17	L	1502	CLA	MG-NB	3.61	2.13	2.05
17	P	5124	CLA	MG-NA	3.60	2.17	2.07
17	Q	5130	CLA	MG-NA	3.57	2.17	2.07
17	Q	5214	CLA	MG-NB	3.57	2.13	2.05
17	Q	5237	CLA	MG-NA	3.57	2.17	2.07
17	Q	5239	CLA	MG-NA	3.57	2.17	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1237	CLA	MG-NA	3.57	2.17	2.07
17	B	1239	CLA	MG-NA	3.56	2.17	2.07
17	B	1235	CLA	MG-NA	3.56	2.17	2.07
17	A	1124	CLA	MG-NA	3.56	2.17	2.07
17	B	1214	CLA	MG-NB	3.55	2.12	2.05
17	A	1102	CLA	C4A-NA	-3.55	1.35	1.38
17	Q	5235	CLA	MG-NA	3.54	2.17	2.07
17	B	1130	CLA	MG-NA	3.54	2.17	2.07
17	A	1122	CLA	C4A-NA	-3.50	1.35	1.38
17	A	1901	CLA	C1C-NC	-3.49	1.33	1.39
17	F	1301	CLA	C4A-NA	-3.49	1.35	1.38
17	P	5901	CLA	C1C-NC	-3.48	1.33	1.39
17	B	1239	CLA	C4A-NA	-3.45	1.35	1.38
17	Q	5239	CLA	C4A-NA	-3.45	1.35	1.38
17	P	5102	CLA	C4A-NA	-3.44	1.35	1.38
17	P	5122	CLA	C4A-NA	-3.43	1.35	1.38
17	A	1108	CLA	MG-NC	3.43	2.17	2.07
19	C	3002	SF4	S2-FE3	3.42	2.35	2.33
17	5	5401	CLA	MG-NB	3.42	2.12	2.05
17	K	1401	CLA	MG-NB	3.42	2.12	2.05
17	P	5108	CLA	MG-NC	3.41	2.17	2.07
17	P	5113	CLA	C4A-NA	-3.41	1.35	1.38
17	P	5105	CLA	MG-NB	3.41	2.12	2.05
17	A	1105	CLA	MG-NB	3.40	2.12	2.05
17	B	1231	CLA	MG-NB	3.39	2.12	2.05
17	Q	5231	CLA	MG-NB	3.39	2.12	2.05
17	U	5301	CLA	C4A-NA	-3.39	1.35	1.38
17	Q	5204	CLA	MG-NA	3.38	2.17	2.07
17	A	1139	CLA	C4A-NA	-3.38	1.35	1.38
17	A	1012	CLA	MG-NB	3.37	2.12	2.05
17	B	1204	CLA	MG-NA	3.37	2.17	2.07
17	A	1113	CLA	C4A-NA	-3.37	1.35	1.38
18	P	6001	PQN	C10-C5	3.37	1.45	1.40
18	A	2001	PQN	C10-C5	3.36	1.45	1.40
17	A	1137	CLA	C1C-NC	-3.35	1.34	1.39
17	P	5012	CLA	MG-NB	3.34	2.12	2.05
17	P	5137	CLA	C1C-NC	-3.32	1.34	1.39
17	9	1022	CLA	MG-NB	3.31	2.12	2.05
19	R	7002	SF4	S2-FE3	3.31	2.35	2.33
17	B	1230	CLA	MG-NB	3.31	2.12	2.05
17	P	5139	CLA	C4A-NA	-3.31	1.35	1.38
17	B	1022	CLA	MG-NC	3.30	2.17	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	0	1015	CLA	MG-NB	3.30	2.12	2.05
17	Q	5230	CLA	MG-NB	3.30	2.12	2.05
17	0	1011	CLA	MG-NB	3.30	2.12	2.05
17	Q	5022	CLA	MG-NC	3.29	2.17	2.07
17	A	1111	CLA	MG-NB	3.29	2.12	2.05
17	0	1012	CLA	MG-NB	3.29	2.12	2.05
17	7	1015	CLA	MG-NB	3.29	2.12	2.05
17	5	5403	CLA	MG-NB	3.28	2.12	2.05
17	1	1022	CLA	MG-NB	3.28	2.12	2.05
17	8	1012	CLA	MG-NB	3.28	2.12	2.05
17	4	1022	CLA	MG-NB	3.28	2.12	2.05
19	C	3003	SF4	S3-FE1	-3.28	2.31	2.33
17	P	5111	CLA	MG-NB	3.27	2.12	2.05
17	K	1403	CLA	MG-NB	3.27	2.12	2.05
17	8	1033	CLA	MG-NB	3.27	2.12	2.05
17	P	8010	CLA	MG-NB	3.27	2.12	2.05
17	7	1022	CLA	MG-NB	3.27	2.12	2.05
17	9	1012	CLA	MG-NB	3.27	2.12	2.05
17	3	1033	CLA	MG-NB	3.27	2.12	2.05
17	9	1033	CLA	MG-NB	3.27	2.12	2.05
17	9	1014	CLA	MG-NB	3.27	2.12	2.05
17	3	1022	CLA	MG-NB	3.27	2.12	2.05
17	4	1012	CLA	MG-NB	3.26	2.12	2.05
17	L	1501	CLA	MG-NB	3.26	2.12	2.05
17	4	1011	CLA	MG-NB	3.26	2.12	2.05
17	1	1015	CLA	MG-NB	3.26	2.12	2.05
17	7	1023	CLA	MG-NB	3.26	2.12	2.05
17	A	4010	CLA	MG-NB	3.26	2.12	2.05
17	A	4009	CLA	MG-NB	3.26	2.12	2.05
17	0	1022	CLA	MG-NB	3.26	2.12	2.05
17	7	1012	CLA	MG-NB	3.26	2.12	2.05
17	Q	5212	CLA	MG-NB	3.26	2.12	2.05
17	2	1025	CLA	MG-NB	3.26	2.12	2.05
17	4	1015	CLA	MG-NB	3.25	2.12	2.05
17	B	1219	CLA	C1C-NC	-3.25	1.34	1.39
17	8	1015	CLA	MG-NB	3.25	2.12	2.05
17	8	1011	CLA	MG-NB	3.25	2.12	2.05
17	3	1012	CLA	MG-NB	3.25	2.12	2.05
17	K	1404	CLA	MG-NB	3.25	2.12	2.05
17	0	1023	CLA	MG-NB	3.25	2.12	2.05
17	5	5404	CLA	MG-NB	3.25	2.12	2.05
17	9	1016	CLA	MG-NB	3.24	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	1023	CLA	MG-NB	3.25	2.12	2.05
17	P	8009	CLA	MG-NB	3.24	2.12	2.05
17	2	1021	CLA	MG-NB	3.24	2.12	2.05
17	3	1016	CLA	MG-NB	3.24	2.12	2.05
17	6	5501	CLA	MG-NB	3.24	2.12	2.05
17	B	1212	CLA	MG-NB	3.24	2.12	2.05
17	0	1017	CLA	MG-NB	3.24	2.12	2.05
17	4	1026	CLA	MG-NB	3.24	2.12	2.05
17	3	1031	CLA	MG-NB	3.24	2.12	2.05
17	4	1031	CLA	MG-NB	3.24	2.12	2.05
17	7	1013	CLA	MG-NB	3.24	2.12	2.05
17	3	1014	CLA	MG-NB	3.24	2.12	2.05
17	2	1033	CLA	MG-NB	3.24	2.12	2.05
17	2	1015	CLA	MG-NB	3.24	2.12	2.05
17	2	4007	CLA	MG-NB	3.24	2.12	2.05
17	2	1023	CLA	MG-NB	3.24	2.12	2.05
17	0	1031	CLA	MG-NB	3.24	2.12	2.05
17	F	4003	CLA	MG-NB	3.24	2.12	2.05
17	1	1012	CLA	MG-NB	3.23	2.12	2.05
17	1	1023	CLA	MG-NB	3.23	2.12	2.05
17	Q	8001	CLA	MG-NB	3.23	2.12	2.05
17	9	1015	CLA	MG-NB	3.23	2.12	2.05
17	4	1017	CLA	MG-NB	3.23	2.12	2.05
17	3	1041	CLA	MG-NB	3.23	2.12	2.05
17	W	5801	CLA	MG-NB	3.23	2.12	2.05
17	8	1013	CLA	MG-NB	3.23	2.12	2.05
17	7	1025	CLA	MG-NB	3.23	2.12	2.05
17	7	1026	CLA	MG-NB	3.23	2.12	2.05
17	9	1011	CLA	MG-NB	3.23	2.12	2.05
17	Q	5208	CLA	MG-NB	3.23	2.12	2.05
17	L	1504	CLA	MG-NB	3.23	2.12	2.05
17	U	8003	CLA	MG-NB	3.23	2.12	2.05
17	8	1023	CLA	MG-NB	3.23	2.12	2.05
17	2	1013	CLA	MG-NB	3.23	2.12	2.05
17	6	5504	CLA	MG-NB	3.23	2.12	2.05
17	2	1012	CLA	MG-NB	3.23	2.12	2.05
17	3	1015	CLA	MG-NB	3.23	2.12	2.05
17	8	1025	CLA	MG-NB	3.23	2.12	2.05
17	8	1021	CLA	MG-NB	3.23	2.12	2.05
19	R	7003	SF4	S3-FE1	-3.23	2.31	2.33
17	4	1025	CLA	MG-NB	3.23	2.12	2.05
17	1	1025	CLA	MG-NB	3.23	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1241	CLA	MG-NB	3.23	2.12	2.05
17	Q	5241	CLA	MG-NB	3.23	2.12	2.05
17	1	1017	CLA	MG-NB	3.23	2.12	2.05
17	8	8007	CLA	MG-NB	3.23	2.12	2.05
17	7	1017	CLA	MG-NB	3.22	2.12	2.05
17	9	1031	CLA	MG-NB	3.23	2.12	2.05
17	J	1101	CLA	MG-NB	3.23	2.12	2.05
17	8	1016	CLA	MG-NB	3.23	2.12	2.05
17	3	1032	CLA	MG-NB	3.23	2.12	2.05
17	9	1026	CLA	MG-NB	3.22	2.12	2.05
17	0	1026	CLA	MG-NB	3.22	2.12	2.05
17	9	1041	CLA	MG-NB	3.22	2.12	2.05
17	B	1226	CLA	MG-NB	3.22	2.12	2.05
17	9	1032	CLA	MG-NB	3.22	2.12	2.05
17	2	1011	CLA	MG-NB	3.22	2.12	2.05
17	1	1026	CLA	MG-NB	3.22	2.12	2.05
17	2	1026	CLA	MG-NB	3.22	2.12	2.05
17	3	1011	CLA	MG-NB	3.22	2.12	2.05
17	9	1017	CLA	MG-NB	3.22	2.12	2.05
17	4	1033	CLA	MG-NB	3.22	2.12	2.05
17	1	1013	CLA	MG-NB	3.22	2.12	2.05
17	3	1026	CLA	MG-NB	3.22	2.12	2.05
17	2	1016	CLA	MG-NB	3.22	2.12	2.05
17	B	1242	CLA	MG-NB	3.22	2.12	2.05
17	0	1033	CLA	MG-NB	3.22	2.12	2.05
17	7	1031	CLA	MG-NB	3.22	2.12	2.05
17	7	1016	CLA	MG-NB	3.22	2.12	2.05
17	G	1701	CLA	MG-NB	3.22	2.12	2.05
17	1	1011	CLA	MG-NB	3.22	2.12	2.05
17	8	1026	CLA	MG-NB	3.22	2.12	2.05
17	2	1014	CLA	MG-NB	3.22	2.12	2.05
17	Q	5219	CLA	C1C-NC	-3.21	1.34	1.39
17	F	4006	CLA	MG-NB	3.21	2.12	2.05
17	7	1011	CLA	MG-NB	3.21	2.12	2.05
17	3	1021	CLA	MG-NB	3.21	2.12	2.05
17	4	1013	CLA	MG-NB	3.21	2.12	2.05
17	U	8004	CLA	MG-NB	3.21	2.12	2.05
17	2	1017	CLA	MG-NB	3.21	2.12	2.05
17	F	4004	CLA	MG-NB	3.21	2.12	2.05
17	J	4008	CLA	MG-NB	3.21	2.12	2.05
17	4	1021	CLA	MG-NB	3.21	2.12	2.05
17	B	4001	CLA	MG-NB	3.21	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	1016	CLA	MG-NB	3.21	2.12	2.05
17	Q	5226	CLA	MG-NB	3.21	2.12	2.05
17	U	8005	CLA	MG-NB	3.21	2.12	2.05
17	3	1025	CLA	MG-NB	3.21	2.12	2.05
17	4	1016	CLA	MG-NB	3.20	2.12	2.05
17	B	1208	CLA	MG-NB	3.20	2.12	2.05
17	4	1032	CLA	MG-NB	3.20	2.12	2.05
17	0	1016	CLA	MG-NB	3.20	2.12	2.05
17	0	1025	CLA	MG-NB	3.20	2.12	2.05
17	H	1801	CLA	MG-NB	3.20	2.12	2.05
17	Z	5101	CLA	MG-NB	3.20	2.12	2.05
17	1	1031	CLA	MG-NB	3.20	2.12	2.05
17	4	4002	CLA	MG-NB	3.20	2.12	2.05
17	Q	5242	CLA	MG-NB	3.20	2.12	2.05
17	4	1014	CLA	MG-NB	3.20	2.12	2.05
17	V	5701	CLA	MG-NB	3.20	2.12	2.05
17	8	1014	CLA	MG-NB	3.20	2.12	2.05
17	8	1017	CLA	MG-NB	3.20	2.12	2.05
17	1	1014	CLA	MG-NB	3.20	2.12	2.05
17	0	1013	CLA	MG-NB	3.20	2.12	2.05
17	B	1240	CLA	MG-NB	3.20	2.12	2.05
17	9	1021	CLA	MG-NB	3.19	2.12	2.05
17	0	1014	CLA	MG-NB	3.19	2.12	2.05
17	3	1017	CLA	MG-NB	3.19	2.12	2.05
17	F	4005	CLA	MG-NB	3.19	2.12	2.05
17	Q	5240	CLA	MG-NB	3.19	2.12	2.05
17	P	5126	CLA	C1C-NC	-3.19	1.34	1.39
17	0	1021	CLA	MG-NB	3.19	2.12	2.05
17	Z	8008	CLA	MG-NB	3.19	2.12	2.05
17	U	8006	CLA	MG-NB	3.19	2.12	2.05
17	Q	5235	CLA	MG-NB	3.19	2.12	2.05
17	2	1031	CLA	MG-NB	3.19	2.12	2.05
17	7	1014	CLA	MG-NB	3.18	2.12	2.05
17	P	5123	CLA	MG-NB	3.18	2.12	2.05
17	A	1138	CLA	MG-NB	3.18	2.12	2.05
17	0	8002	CLA	MG-NB	3.18	2.12	2.05
17	A	1123	CLA	MG-NB	3.18	2.12	2.05
17	9	1025	CLA	MG-NB	3.18	2.12	2.05
17	2	1022	CLA	MG-NB	3.18	2.12	2.05
17	8	1031	CLA	MG-NB	3.18	2.12	2.05
17	A	1126	CLA	C1C-NC	-3.18	1.34	1.39
17	0	1032	CLA	MG-NB	3.17	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1235	CLA	MG-NB	3.17	2.12	2.05
17	P	5138	CLA	MG-NB	3.17	2.12	2.05
17	G	1233	CLA	C4A-NA	-3.16	1.35	1.38
17	Q	5220	CLA	MG-NB	3.16	2.12	2.05
17	8	1022	CLA	MG-NB	3.16	2.12	2.05
17	B	1224	CLA	MG-NC	3.15	2.16	2.07
17	L	1503	CLA	MG-NB	3.14	2.12	2.05
17	B	1220	CLA	MG-NB	3.15	2.12	2.05
17	Q	5224	CLA	MG-NC	3.13	2.16	2.07
17	B	1209	CLA	MG-NB	3.13	2.12	2.05
17	6	5503	CLA	MG-NB	3.13	2.12	2.05
17	Q	5209	CLA	MG-NB	3.12	2.12	2.05
17	5	5401	CLA	C4A-NA	-3.12	1.35	1.38
17	B	1239	CLA	C1C-NC	-3.12	1.34	1.39
17	Q	5239	CLA	C1C-NC	-3.12	1.34	1.39
17	K	1401	CLA	C4A-NA	-3.12	1.35	1.38
17	Q	5235	CLA	CHC-C1C	3.11	1.45	1.37
17	B	1235	CLA	CHC-C1C	3.11	1.45	1.37
17	Q	5236	CLA	MG-NB	3.08	2.11	2.05
17	Q	5218	CLA	MG-NB	3.07	2.11	2.05
17	V	5233	CLA	C4A-NA	-3.07	1.35	1.38
17	F	1301	CLA	MG-NB	3.07	2.11	2.05
17	U	5301	CLA	MG-NB	3.07	2.11	2.05
17	B	1236	CLA	MG-NB	3.06	2.11	2.05
19	C	3002	SF4	S3-FE2	3.06	2.35	2.33
17	P	5139	CLA	MG-NB	3.05	2.11	2.05
17	P	5116	CLA	MG-NB	3.05	2.11	2.05
17	B	1218	CLA	MG-NB	3.05	2.11	2.05
17	P	5140	CLA	C4A-NA	-3.04	1.35	1.38
17	A	1139	CLA	MG-NB	3.03	2.11	2.05
17	A	1109	CLA	MG-NB	3.02	2.11	2.05
17	A	1116	CLA	MG-NB	3.02	2.11	2.05
17	B	1216	CLA	C4A-NA	-3.02	1.35	1.38
17	P	5109	CLA	MG-NB	3.02	2.11	2.05
17	L	1501	CLA	CHC-C1C	3.01	1.45	1.37
17	P	5113	CLA	C1C-NC	-3.01	1.34	1.39
17	A	1121	CLA	MG-NB	3.01	2.11	2.05
19	R	7002	SF4	S3-FE2	3.01	2.35	2.33
17	P	5121	CLA	MG-NB	3.00	2.11	2.05
17	6	5501	CLA	CHC-C1C	3.00	1.44	1.37
17	P	5114	CLA	C4A-NA	-3.00	1.35	1.38
17	Q	5023	CLA	MG-NB	2.99	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1136	CLA	C4A-NA	-2.99	1.35	1.38
17	B	1225	CLA	MG-NB	2.99	2.11	2.05
17	B	1023	CLA	MG-NB	2.99	2.11	2.05
17	B	1201	CLA	MG-NB	2.99	2.11	2.05
17	Q	5023	CLA	CHC-C1C	2.98	1.44	1.37
17	Q	5225	CLA	MG-NB	2.98	2.11	2.05
17	Q	5201	CLA	MG-NB	2.98	2.11	2.05
17	P	5136	CLA	C4A-NA	-2.98	1.35	1.38
17	A	1113	CLA	C1C-NC	-2.98	1.34	1.39
17	Q	5205	CLA	C4A-NA	-2.97	1.35	1.38
18	B	2002	PQN	C6-C5	2.97	1.44	1.39
17	B	1205	CLA	C4A-NA	-2.97	1.35	1.38
17	B	1023	CLA	CHC-C1C	2.97	1.44	1.37
17	Q	5218	CLA	CHC-C1C	2.96	1.44	1.37
17	Z	5302	CLA	C1C-NC	-2.96	1.34	1.39
18	Q	6002	PQN	C6-C5	2.96	1.44	1.39
17	B	1218	CLA	CHC-C1C	2.96	1.44	1.37
17	A	1140	CLA	C4A-NA	-2.94	1.36	1.38
17	J	1302	CLA	C1C-NC	-2.94	1.34	1.39
17	B	1218	CLA	C4A-NA	-2.93	1.36	1.38
17	A	1128	CLA	CHC-C1C	2.92	1.44	1.37
17	J	1302	CLA	MG-NC	2.92	2.15	2.07
17	Q	5216	CLA	C4A-NA	-2.92	1.36	1.38
17	A	1012	CLA	MG-NC	2.91	2.15	2.07
17	Z	5302	CLA	MG-NC	2.91	2.15	2.07
17	P	5128	CLA	CHC-C1C	2.90	1.44	1.37
17	P	5105	CLA	C4A-NA	-2.90	1.36	1.38
17	A	1126	CLA	MG-NC	2.89	2.15	2.07
17	P	5012	CLA	MG-NC	2.89	2.15	2.07
17	B	1217	CLA	MG-NB	2.89	2.11	2.05
17	A	1134	CLA	MG-NB	2.89	2.11	2.05
17	P	5126	CLA	MG-NC	2.89	2.15	2.07
17	B	1217	CLA	C4A-NA	-2.88	1.36	1.38
17	A	1114	CLA	C4A-NA	-2.88	1.36	1.38
17	Q	5238	CLA	C1C-NC	-2.88	1.34	1.39
17	B	1238	CLA	C1C-NC	-2.87	1.34	1.39
17	Q	5217	CLA	MG-NB	2.86	2.11	2.05
17	A	1105	CLA	C4A-NA	-2.86	1.36	1.38
17	P	5901	CLA	MG-NC	2.86	2.15	2.07
18	P	6001	PQN	C6-C5	2.86	1.44	1.39
18	A	2001	PQN	C6-C5	2.86	1.44	1.39
17	A	1901	CLA	CHC-C1C	2.85	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5901	CLA	CHC-C1C	2.85	1.44	1.37
17	P	5134	CLA	MG-NB	2.85	2.11	2.05
17	A	1901	CLA	MG-NC	2.85	2.15	2.07
17	6	5502	CLA	CHC-C1C	2.85	1.44	1.37
17	Q	5218	CLA	C4A-NA	-2.84	1.36	1.38
17	P	5131	CLA	C1C-NC	-2.85	1.34	1.39
17	L	1502	CLA	CHC-C1C	2.84	1.44	1.37
17	B	1211	CLA	MG-NB	2.84	2.11	2.05
17	A	1131	CLA	C1C-NC	-2.84	1.34	1.39
17	P	5106	CLA	C1C-NC	-2.84	1.34	1.39
17	P	5113	CLA	MG-NC	2.83	2.15	2.07
17	P	5138	CLA	CHC-C1C	2.83	1.44	1.37
17	A	1138	CLA	CHC-C1C	2.83	1.44	1.37
17	B	1023	CLA	C1D-CHD	2.83	1.44	1.36
17	P	5106	CLA	CHC-C1C	2.83	1.44	1.37
17	P	5110	CLA	C4A-NA	-2.83	1.36	1.38
17	Q	5211	CLA	MG-NB	2.82	2.11	2.05
17	A	1106	CLA	C1C-NC	-2.82	1.35	1.39
17	P	5120	CLA	MG-NB	2.82	2.11	2.05
17	A	1113	CLA	MG-NC	2.81	2.15	2.07
17	Q	5023	CLA	C1D-CHD	2.81	1.44	1.36
17	P	5118	CLA	MG-NB	2.81	2.11	2.05
17	A	1106	CLA	CHC-C1C	2.81	1.44	1.37
17	A	1118	CLA	MG-NB	2.80	2.11	2.05
17	B	1221	CLA	CHC-C1C	2.80	1.44	1.37
17	G	1233	CLA	MG-NB	2.79	2.11	2.05
17	A	1120	CLA	MG-NB	2.79	2.11	2.05
17	A	1112	CLA	MG-NB	2.79	2.11	2.05
17	A	1112	CLA	CHC-C1C	2.79	1.44	1.37
17	Q	5217	CLA	C4A-NA	-2.79	1.36	1.38
17	Q	5021	CLA	MG-NB	2.78	2.11	2.05
17	P	5112	CLA	CHC-C1C	2.78	1.44	1.37
17	P	5112	CLA	MG-NB	2.78	2.11	2.05
17	Q	5221	CLA	CHC-C1C	2.78	1.44	1.37
17	B	1021	CLA	MG-NB	2.78	2.11	2.05
17	B	1224	CLA	CHC-C1C	2.78	1.44	1.37
17	V	5233	CLA	MG-NB	2.78	2.11	2.05
17	P	5125	CLA	CHC-C1C	2.78	1.44	1.37
17	Q	5224	CLA	CHC-C1C	2.77	1.44	1.37
17	Q	5231	CLA	CHC-C1C	2.77	1.44	1.37
17	B	1206	CLA	MG-NC	2.77	2.15	2.07
17	B	1231	CLA	CHC-C1C	2.77	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5206	CLA	MG-NC	2.76	2.15	2.07
17	A	1125	CLA	CHC-C1C	2.76	1.44	1.37
17	Q	5204	CLA	C1D-CHD	2.76	1.43	1.36
17	Q	5224	CLA	MG-NB	2.75	2.11	2.05
17	Q	5212	CLA	CHC-C1C	2.75	1.44	1.37
17	B	1224	CLA	MG-NB	2.75	2.11	2.05
17	A	1140	CLA	C1C-NC	-2.75	1.35	1.39
17	B	1204	CLA	C1D-CHD	2.74	1.43	1.36
17	B	1212	CLA	CHC-C1C	2.74	1.44	1.37
17	A	1102	CLA	MG-NB	2.73	2.11	2.05
17	Q	5232	CLA	CHC-C1C	2.73	1.44	1.37
17	B	1213	CLA	C4A-NA	-2.73	1.36	1.38
17	P	5102	CLA	MG-NB	2.72	2.11	2.05
17	A	1124	CLA	MG-NB	2.72	2.11	2.05
17	B	1232	CLA	CHC-C1C	2.72	1.44	1.37
17	B	1213	CLA	MG-NB	2.72	2.11	2.05
17	P	5140	CLA	C1C-NC	-2.72	1.35	1.39
17	Q	5220	CLA	CHC-C1C	2.72	1.44	1.37
17	P	5118	CLA	CHC-C1C	2.72	1.44	1.37
17	B	1209	CLA	C4A-NA	-2.72	1.36	1.38
17	B	1220	CLA	CHC-C1C	2.72	1.44	1.37
17	Q	5234	CLA	CHC-C1C	2.72	1.44	1.37
17	P	5123	CLA	CHC-C1C	2.71	1.44	1.37
17	P	5119	CLA	CHC-C1C	2.71	1.44	1.37
17	P	5124	CLA	MG-NB	2.71	2.11	2.05
17	A	1110	CLA	C4A-NA	-2.71	1.36	1.38
17	A	1119	CLA	CHC-C1C	2.71	1.44	1.37
17	Q	5213	CLA	MG-NB	2.70	2.11	2.05
17	P	5117	CLA	MG-NB	2.70	2.11	2.05
17	P	5126	CLA	MG-NB	2.69	2.11	2.05
17	Q	5220	CLA	C4A-NA	-2.70	1.36	1.38
17	A	1118	CLA	CHC-C1C	2.69	1.44	1.37
17	6	5503	CLA	CHC-C1C	2.69	1.44	1.37
17	B	1234	CLA	CHC-C1C	2.69	1.44	1.37
17	A	1123	CLA	CHC-C1C	2.68	1.44	1.37
17	A	1106	CLA	MG-NB	2.68	2.11	2.05
17	Q	5203	CLA	C1D-CHD	2.68	1.43	1.36
17	P	5106	CLA	MG-NB	2.67	2.11	2.05
17	A	1117	CLA	MG-NB	2.67	2.11	2.05
17	Q	5222	CLA	MG-NB	2.67	2.10	2.05
17	A	1126	CLA	MG-NB	2.67	2.10	2.05
17	Q	5238	CLA	C4A-NA	-2.67	1.36	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	1503	CLA	CHC-C1C	2.66	1.44	1.37
17	B	1220	CLA	C4A-NA	-2.66	1.36	1.38
17	Q	5213	CLA	C4A-NA	-2.66	1.36	1.38
17	B	1238	CLA	C4A-NA	-2.66	1.36	1.38
17	B	1203	CLA	C1D-CHD	2.65	1.43	1.36
17	A	1120	CLA	CHC-C1C	2.65	1.44	1.37
17	P	5120	CLA	CHC-C1C	2.65	1.44	1.37
17	B	1215	CLA	MG-NB	2.64	2.10	2.05
17	P	5012	CLA	CHC-C1C	2.64	1.44	1.37
17	Q	5209	CLA	C4A-NA	-2.64	1.36	1.38
17	P	5124	CLA	C1C-NC	-2.64	1.35	1.39
17	Q	5215	CLA	MG-NB	2.63	2.10	2.05
17	A	1012	CLA	CHC-C1C	2.63	1.44	1.37
17	Q	5232	CLA	MG-NB	2.63	2.10	2.05
17	A	1121	CLA	C1D-CHD	2.62	1.43	1.36
17	U	5229	CLA	MG-NB	2.62	2.10	2.05
17	B	1222	CLA	MG-NB	2.62	2.10	2.05
17	J	1302	CLA	CHC-C1C	2.62	1.44	1.37
17	P	5121	CLA	C1D-CHD	2.61	1.43	1.36
17	A	1124	CLA	C1C-NC	-2.61	1.35	1.39
17	B	1232	CLA	MG-NB	2.60	2.10	2.05
17	Q	5227	CLA	MG-NB	2.60	2.10	2.05
17	A	1129	CLA	CHC-C1C	2.60	1.43	1.37
17	Z	5302	CLA	CHC-C1C	2.60	1.43	1.37
17	A	1136	CLA	CHC-C1C	2.59	1.43	1.37
17	F	1229	CLA	MG-NB	2.59	2.10	2.05
17	B	1227	CLA	MG-NB	2.59	2.10	2.05
17	Q	5228	CLA	CHC-C1C	2.58	1.43	1.37
17	P	5129	CLA	CHC-C1C	2.58	1.43	1.37
17	B	1228	CLA	CHC-C1C	2.58	1.43	1.37
17	P	5110	CLA	C1D-CHD	2.58	1.43	1.36
17	P	5102	CLA	CHC-C1C	2.57	1.43	1.37
17	P	5136	CLA	CHC-C1C	2.58	1.43	1.37
17	A	1110	CLA	C1D-CHD	2.57	1.43	1.36
17	A	1102	CLA	CHC-C1C	2.57	1.43	1.37
17	P	5137	CLA	CHC-C1C	2.56	1.43	1.37
17	A	1137	CLA	CHC-C1C	2.56	1.43	1.37
17	U	5301	CLA	CHC-C1C	2.56	1.43	1.37
17	A	1140	CLA	CHC-C1C	2.56	1.43	1.37
17	B	1219	CLA	MG-NC	2.56	2.14	2.07
17	F	1301	CLA	CHC-C1C	2.55	1.43	1.37
17	Q	5228	CLA	MG-NB	2.55	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1228	CLA	MG-NB	2.54	2.10	2.05
17	P	5140	CLA	CHC-C1C	2.54	1.43	1.37
18	A	2001	PQN	C10-C1	-2.54	1.43	1.48
18	P	6001	PQN	C10-C1	-2.54	1.43	1.48
17	A	1115	CLA	C4A-NA	-2.54	1.36	1.38
17	P	5102	CLA	C1C-NC	-2.53	1.35	1.39
17	Q	5219	CLA	MG-NC	2.53	2.14	2.07
17	B	1209	CLA	C1D-CHD	2.53	1.43	1.36
17	Q	5231	CLA	C1D-CHD	2.53	1.43	1.36
17	P	5128	CLA	C4A-NA	-2.52	1.36	1.38
17	Q	5209	CLA	C1D-CHD	2.52	1.43	1.36
17	A	1102	CLA	C1C-NC	-2.52	1.35	1.39
17	B	1201	CLA	CHC-C1C	2.52	1.43	1.37
17	B	1204	CLA	MG-NB	2.51	2.10	2.05
17	B	1216	CLA	MG-NB	2.51	2.10	2.05
17	P	5114	CLA	MG-NB	2.51	2.10	2.05
17	B	1221	CLA	C1D-CHD	2.50	1.43	1.36
17	B	1021	CLA	MG-NC	2.50	2.14	2.07
17	Q	5204	CLA	MG-NB	2.50	2.10	2.05
17	Q	5221	CLA	C1D-CHD	2.50	1.43	1.36
17	P	5122	CLA	C1C-NC	-2.49	1.35	1.39
17	J	1302	CLA	C1D-CHD	2.50	1.43	1.36
17	A	1122	CLA	C1C-NC	-2.49	1.35	1.39
17	Z	5302	CLA	C1D-CHD	2.49	1.43	1.36
17	B	1231	CLA	C1D-CHD	2.49	1.43	1.36
17	A	1114	CLA	MG-NB	2.49	2.10	2.05
17	Q	5201	CLA	CHC-C1C	2.49	1.43	1.37
17	A	1110	CLA	MG-NB	2.49	2.10	2.05
17	Q	5216	CLA	MG-NB	2.48	2.10	2.05
17	A	1103	CLA	CHC-C1C	2.48	1.43	1.37
17	P	5122	CLA	MG-NB	2.48	2.10	2.05
17	P	5110	CLA	MG-NB	2.48	2.10	2.05
17	Q	5223	CLA	CHC-C1C	2.48	1.43	1.37
17	A	1122	CLA	MG-NB	2.47	2.10	2.05
17	B	1223	CLA	CHC-C1C	2.47	1.43	1.37
17	Q	5021	CLA	MG-NC	2.47	2.14	2.07
17	A	1133	CLA	C1C-NC	-2.47	1.35	1.39
17	P	5115	CLA	C4A-NA	-2.47	1.36	1.38
17	P	5103	CLA	CHC-C1C	2.46	1.43	1.37
17	A	1128	CLA	C4A-NA	-2.46	1.36	1.38
17	B	1214	CLA	CHC-C1C	2.46	1.43	1.37
17	P	5105	CLA	CHC-C1C	2.46	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1105	CLA	CHC-C1C	2.46	1.43	1.37
17	P	5123	CLA	C1D-CHD	2.46	1.43	1.36
17	A	1123	CLA	C1D-CHD	2.45	1.43	1.36
17	P	5127	CLA	C1D-CHD	2.45	1.43	1.36
17	P	5139	CLA	C1C-NC	-2.45	1.35	1.39
17	Q	5214	CLA	CHC-C1C	2.45	1.43	1.37
17	P	5119	CLA	C1D-CHD	2.45	1.43	1.36
17	A	1136	CLA	C1D-CHD	2.45	1.43	1.36
17	P	5136	CLA	C1D-CHD	2.44	1.43	1.36
17	A	1127	CLA	C1D-CHD	2.43	1.43	1.36
17	Q	5239	CLA	MG-NB	2.43	2.10	2.05
17	B	1210	CLA	MG-NC	2.42	2.14	2.07
17	A	1116	CLA	CHC-C1C	2.42	1.43	1.37
17	P	5119	CLA	MG-NB	2.42	2.10	2.05
17	A	1119	CLA	C1D-CHD	2.42	1.42	1.36
17	B	1239	CLA	MG-NB	2.42	2.10	2.05
17	A	1135	CLA	MG-NC	2.42	2.14	2.07
17	P	5140	CLA	MG-NB	2.42	2.10	2.05
17	P	5116	CLA	CHC-C1C	2.42	1.43	1.37
17	P	5135	CLA	MG-NC	2.41	2.14	2.07
17	P	5133	CLA	C1C-NC	-2.41	1.35	1.39
17	Q	5228	CLA	C1B-CHB	-2.41	1.32	1.40
17	Q	5237	CLA	MG-NB	2.41	2.10	2.05
17	A	1127	CLA	MG-NB	2.41	2.10	2.05
17	B	1237	CLA	MG-NB	2.41	2.10	2.05
17	Q	5222	CLA	C1D-CHD	2.41	1.42	1.36
17	P	5127	CLA	MG-NB	2.41	2.10	2.05
17	A	1140	CLA	MG-NB	2.41	2.10	2.05
17	B	1207	CLA	C1C-NC	-2.41	1.35	1.39
17	A	1139	CLA	C1C-NC	-2.40	1.35	1.39
17	B	1228	CLA	C1B-CHB	-2.40	1.32	1.40
17	B	1210	CLA	C1D-CHD	2.40	1.42	1.36
18	B	2002	PQN	C9-C10	2.40	1.43	1.39
17	P	5120	CLA	C1D-CHD	2.40	1.42	1.36
17	A	1120	CLA	C1D-CHD	2.39	1.42	1.36
17	Q	5210	CLA	MG-NC	2.39	2.14	2.07
17	B	1226	CLA	MG-NC	2.39	2.14	2.07
17	B	1222	CLA	C1D-CHD	2.39	1.42	1.36
17	A	1119	CLA	MG-NB	2.39	2.10	2.05
17	B	1205	CLA	C1B-CHB	-2.39	1.32	1.40
17	Q	5205	CLA	C1B-CHB	-2.39	1.32	1.40
17	Q	5023	CLA	MG-NC	2.39	2.14	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5022	CLA	C1D-CHD	2.39	1.42	1.36
17	F	1229	CLA	CHC-C1C	2.39	1.43	1.37
17	Q	5226	CLA	C1D-CHD	2.39	1.42	1.36
17	A	1127	CLA	MG-NC	2.38	2.14	2.07
17	Q	5207	CLA	C1C-NC	-2.38	1.35	1.39
17	B	1023	CLA	MG-NC	2.38	2.14	2.07
17	Q	5210	CLA	C1D-CHD	2.38	1.42	1.36
17	P	5118	CLA	C1C-NC	-2.38	1.35	1.39
17	A	1129	CLA	MG-NB	2.37	2.10	2.05
17	B	1226	CLA	C1D-CHD	2.37	1.42	1.36
17	B	1022	CLA	C1D-CHD	2.37	1.42	1.36
17	Q	5217	CLA	CHC-C1C	2.37	1.43	1.37
17	Q	5226	CLA	MG-NC	2.37	2.14	2.07
18	Q	6002	PQN	C9-C10	2.36	1.43	1.39
17	P	5127	CLA	MG-NC	2.36	2.14	2.07
17	B	1227	CLA	CHC-C1C	2.36	1.43	1.37
17	P	5104	CLA	CHC-C1C	2.36	1.43	1.37
17	U	5229	CLA	CHC-C1C	2.36	1.43	1.37
17	B	1217	CLA	CHC-C1C	2.36	1.43	1.37
17	Q	5227	CLA	CHC-C1C	2.36	1.43	1.37
17	P	5134	CLA	CHC-C1C	2.35	1.43	1.37
17	A	1109	CLA	C1C-NC	-2.36	1.35	1.39
17	A	1134	CLA	CHC-C1C	2.35	1.43	1.37
17	A	1118	CLA	C1C-NC	-2.35	1.35	1.39
17	P	5013	CLA	C1B-CHB	-2.34	1.33	1.40
17	Q	5218	CLA	C1D-CHD	2.34	1.42	1.36
17	B	1219	CLA	CHC-C1C	2.34	1.43	1.37
17	B	1218	CLA	C1D-CHD	2.34	1.42	1.36
17	P	5129	CLA	MG-NB	2.34	2.10	2.05
17	A	1104	CLA	CHC-C1C	2.33	1.43	1.37
17	5	5401	CLA	C1D-CHD	2.33	1.42	1.36
17	A	1013	CLA	C1B-CHB	-2.33	1.33	1.40
17	Q	5204	CLA	C1C-NC	-2.33	1.35	1.39
17	P	5113	CLA	C1D-CHD	2.33	1.42	1.36
17	P	5109	CLA	C1C-NC	-2.33	1.35	1.39
17	B	1238	CLA	MG-NB	2.32	2.10	2.05
17	A	1011	CLA	MG-NB	2.32	2.10	2.05
17	K	1401	CLA	C1D-CHD	2.32	1.42	1.36
17	Q	5219	CLA	CHC-C1C	2.32	1.43	1.37
17	B	1236	CLA	MG-NC	2.32	2.14	2.07
17	Q	5236	CLA	MG-NC	2.32	2.14	2.07
17	Q	5208	CLA	C1D-CHD	2.31	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1129	CLA	C1B-CHB	-2.31	1.33	1.40
17	P	5129	CLA	C1B-CHB	-2.31	1.33	1.40
17	A	1113	CLA	C1D-CHD	2.31	1.42	1.36
17	P	5011	CLA	MG-NB	2.31	2.10	2.05
17	A	1132	CLA	MG-NB	2.31	2.10	2.05
17	P	5132	CLA	MG-NB	2.31	2.10	2.05
17	A	1115	CLA	CHC-C1C	2.31	1.43	1.37
17	Q	5238	CLA	MG-NB	2.31	2.10	2.05
17	Q	5213	CLA	C1C-NC	-2.31	1.35	1.39
17	B	1209	CLA	CHC-C1C	2.31	1.43	1.37
17	A	1119	CLA	C1B-CHB	-2.30	1.33	1.40
17	B	1227	CLA	C1D-CHD	2.30	1.42	1.36
17	Q	5209	CLA	CHC-C1C	2.30	1.43	1.37
17	P	5115	CLA	CHC-C1C	2.30	1.43	1.37
17	P	5119	CLA	C1B-CHB	-2.30	1.33	1.40
17	Q	5022	CLA	CHC-C1C	2.30	1.43	1.37
17	B	1208	CLA	C1D-CHD	2.30	1.42	1.36
17	Q	5227	CLA	C1D-CHD	2.30	1.42	1.36
17	B	1230	CLA	C1C-NC	-2.29	1.35	1.39
17	Q	5205	CLA	MG-NC	2.29	2.14	2.07
17	B	1204	CLA	C1C-NC	-2.29	1.35	1.39
17	B	1022	CLA	CHC-C1C	2.28	1.43	1.37
17	A	1107	CLA	MG-NB	2.28	2.10	2.05
17	Q	5023	CLA	C1B-CHB	-2.28	1.33	1.40
17	F	1301	CLA	MG-NC	2.28	2.14	2.07
17	B	1213	CLA	C1C-NC	-2.28	1.35	1.39
17	B	1023	CLA	C1B-CHB	-2.28	1.33	1.40
17	Q	5230	CLA	C1C-NC	-2.28	1.35	1.39
17	Q	5228	CLA	C1D-CHD	2.28	1.42	1.36
17	Q	5130	CLA	MG-NB	2.27	2.10	2.05
17	P	5104	CLA	C1D-CHD	2.27	1.42	1.36
17	B	1225	CLA	MG-NC	2.27	2.13	2.07
17	U	5301	CLA	MG-NC	2.27	2.13	2.07
17	B	1205	CLA	MG-NC	2.26	2.13	2.07
17	B	1130	CLA	MG-NB	2.26	2.10	2.05
17	Q	5204	CLA	C1B-CHB	-2.26	1.33	1.40
17	B	1204	CLA	C1B-CHB	-2.26	1.33	1.40
17	Q	5225	CLA	MG-NC	2.26	2.13	2.07
17	Q	5213	CLA	CHC-C1C	2.26	1.43	1.37
17	B	1236	CLA	CHC-C1C	2.26	1.43	1.37
17	Q	5237	CLA	C1C-NC	-2.26	1.35	1.39
17	P	5114	CLA	C1C-NC	-2.26	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5236	CLA	CHC-C1C	2.26	1.43	1.37
17	A	1114	CLA	C1C-NC	-2.26	1.35	1.39
17	B	1228	CLA	C1D-CHD	2.26	1.42	1.36
17	A	1104	CLA	C1D-CHD	2.25	1.42	1.36
18	A	2001	PQN	C9-C10	2.25	1.43	1.39
17	A	1122	CLA	CHC-C1C	2.25	1.43	1.37
17	P	5107	CLA	MG-NB	2.25	2.10	2.05
17	A	1122	CLA	C1D-CHD	2.25	1.42	1.36
17	P	5107	CLA	CHC-C1C	2.24	1.43	1.37
18	P	6001	PQN	C9-C10	2.24	1.43	1.39
17	B	1211	CLA	C1D-CHD	2.24	1.42	1.36
17	B	1211	CLA	CHC-C1C	2.24	1.43	1.37
17	B	1213	CLA	CHC-C1C	2.24	1.43	1.37
17	P	5124	CLA	C1B-CHB	-2.24	1.33	1.40
17	P	5112	CLA	C1D-CHD	2.23	1.42	1.36
17	A	1107	CLA	CHC-C1C	2.23	1.43	1.37
17	A	1112	CLA	C1D-CHD	2.23	1.42	1.36
17	P	5122	CLA	CHC-C1C	2.23	1.43	1.37
17	A	1105	CLA	MG-NC	2.23	2.13	2.07
17	K	1401	CLA	CHC-C1C	2.23	1.43	1.37
17	B	1216	CLA	CHC-C1C	2.23	1.43	1.37
17	Q	5216	CLA	CHC-C1C	2.23	1.43	1.37
17	Q	5211	CLA	C1D-CHD	2.23	1.42	1.36
17	P	5122	CLA	C1D-CHD	2.22	1.42	1.36
17	A	1124	CLA	C1B-CHB	-2.23	1.33	1.40
17	L	1501	CLA	MG-NC	2.23	2.13	2.07
17	B	1217	CLA	C1D-CHD	2.23	1.42	1.36
17	B	1225	CLA	C1D-CHD	2.22	1.42	1.36
17	A	1121	CLA	C1C-NC	-2.22	1.35	1.39
17	A	1131	CLA	C1D-CHD	2.22	1.42	1.36
17	P	5132	CLA	C1C-NC	-2.22	1.35	1.39
17	P	5131	CLA	C1D-CHD	2.22	1.42	1.36
17	L	1502	CLA	C1B-CHB	-2.22	1.33	1.40
17	Q	5211	CLA	CHC-C1C	2.22	1.43	1.37
17	P	5111	CLA	C1D-CHD	2.22	1.42	1.36
17	P	5105	CLA	MG-NC	2.22	2.13	2.07
17	P	5108	CLA	C1C-NC	-2.22	1.35	1.39
17	Q	5225	CLA	C1D-CHD	2.22	1.42	1.36
17	B	1130	CLA	C1D-CHD	2.22	1.42	1.36
17	6	5502	CLA	C1B-CHB	-2.21	1.33	1.40
17	L	1502	CLA	C1C-NC	-2.21	1.35	1.39
17	B	1237	CLA	C1C-NC	-2.21	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5131	CLA	MG-NB	2.21	2.09	2.05
17	A	1402	CLA	C1D-CHD	2.21	1.42	1.36
17	A	1013	CLA	C1D-CHD	2.20	1.42	1.36
17	Q	5130	CLA	C1D-CHD	2.20	1.42	1.36
17	A	1131	CLA	MG-NB	2.20	2.09	2.05
17	Q	5210	CLA	CHC-C1C	2.20	1.42	1.37
17	A	1108	CLA	C1C-NC	-2.20	1.35	1.39
17	A	1138	CLA	C1B-CHB	-2.20	1.33	1.40
17	6	5501	CLA	MG-NC	2.20	2.13	2.07
17	Q	5217	CLA	C1D-CHD	2.20	1.42	1.36
17	9	1025	CLA	CHC-C1C	2.20	1.42	1.37
17	5	5401	CLA	CHC-C1C	2.20	1.42	1.37
17	B	1021	CLA	C1B-CHB	-2.20	1.33	1.40
17	8	1033	CLA	CHC-C1C	2.20	1.42	1.37
17	P	5138	CLA	C1B-CHB	-2.20	1.33	1.40
17	4	1012	CLA	C1B-CHB	-2.20	1.33	1.40
17	P	5013	CLA	C1D-CHD	2.20	1.42	1.36
17	A	1132	CLA	C1C-NC	-2.19	1.36	1.39
17	P	5121	CLA	C1C-NC	-2.19	1.36	1.39
17	A	1111	CLA	C1D-CHD	2.19	1.42	1.36
17	B	1210	CLA	CHC-C1C	2.19	1.42	1.37
17	B	1214	CLA	C1B-CHB	-2.19	1.33	1.40
17	6	5502	CLA	C1C-NC	-2.19	1.36	1.39
17	P	5402	CLA	C1D-CHD	2.19	1.42	1.36
17	8	1031	CLA	CHC-C1C	2.19	1.42	1.37
17	P	5134	CLA	C1D-CHD	2.19	1.42	1.36
17	A	1013	CLA	C1C-NC	-2.19	1.36	1.39
17	B	1235	CLA	C1D-CHD	2.19	1.42	1.36
17	0	8002	CLA	CHC-C1C	2.19	1.42	1.37
17	Q	5021	CLA	C1B-CHB	-2.18	1.33	1.40
17	P	5901	CLA	C1D-CHD	2.18	1.42	1.36
17	0	1023	CLA	CHC-C1C	2.18	1.42	1.37
17	Q	5215	CLA	C1C-NC	-2.18	1.36	1.39
17	A	1128	CLA	C1D-CHD	2.18	1.42	1.36
17	A	1901	CLA	C1D-CHD	2.18	1.42	1.36
17	0	1012	CLA	C1B-CHB	-2.18	1.33	1.40
17	F	1301	CLA	C1D-CHD	2.18	1.42	1.36
17	Q	5214	CLA	C1B-CHB	-2.18	1.33	1.40
17	7	1026	CLA	CHC-C1C	2.18	1.42	1.37
17	2	1033	CLA	CHC-C1C	2.18	1.42	1.37
17	U	8006	CLA	CHC-C1C	2.18	1.42	1.37
17	B	1208	CLA	C1B-CHB	-2.17	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	1026	CLA	CHC-C1C	2.17	1.42	1.37
17	2	1031	CLA	CHC-C1C	2.17	1.42	1.37
17	B	1208	CLA	CHC-C1C	2.17	1.42	1.37
17	Q	5208	CLA	CHC-C1C	2.17	1.42	1.37
17	7	1017	CLA	CHC-C1C	2.17	1.42	1.37
17	0	1022	CLA	CHC-C1C	2.17	1.42	1.37
17	9	1016	CLA	CHC-C1C	2.17	1.42	1.37
17	B	1242	CLA	CHC-C1C	2.17	1.42	1.37
17	P	5128	CLA	C1D-CHD	2.17	1.42	1.36
17	9	1011	CLA	C1B-CHB	-2.17	1.33	1.40
17	U	5301	CLA	C1D-CHD	2.17	1.42	1.36
17	A	1134	CLA	C1D-CHD	2.17	1.42	1.36
17	Q	5209	CLA	C1C-NC	-2.17	1.36	1.39
17	4	1022	CLA	CHC-C1C	2.17	1.42	1.37
17	9	1014	CLA	CHC-C1C	2.17	1.42	1.37
17	9	1021	CLA	CHC-C1C	2.17	1.42	1.37
17	8	1015	CLA	CHC-C1C	2.17	1.42	1.37
17	3	1025	CLA	CHC-C1C	2.17	1.42	1.37
17	0	1011	CLA	CHC-C1C	2.17	1.42	1.37
17	Q	5208	CLA	C1B-CHB	-2.16	1.33	1.40
17	B	1221	CLA	C1B-CHB	-2.16	1.33	1.40
17	2	1022	CLA	CHC-C1C	2.16	1.42	1.37
17	9	1017	CLA	C1B-CHB	-2.16	1.33	1.40
17	B	1241	CLA	CHC-C1C	2.16	1.42	1.37
17	P	5013	CLA	C1C-NC	-2.16	1.36	1.39
17	0	8002	CLA	C1B-CHB	-2.16	1.33	1.40
17	3	1021	CLA	CHC-C1C	2.16	1.42	1.37
17	2	1014	CLA	CHC-C1C	2.16	1.42	1.37
17	3	1014	CLA	CHC-C1C	2.16	1.42	1.37
17	4	1011	CLA	CHC-C1C	2.16	1.42	1.37
17	A	1110	CLA	C1C-NC	-2.16	1.36	1.39
17	9	1041	CLA	CHC-C1C	2.16	1.42	1.37
17	3	1011	CLA	C1B-CHB	-2.16	1.33	1.40
17	4	1025	CLA	CHC-C1C	2.16	1.42	1.37
17	F	4006	CLA	CHC-C1C	2.16	1.42	1.37
17	Q	5241	CLA	CHC-C1C	2.16	1.42	1.37
17	P	5133	CLA	MG-NB	2.16	2.09	2.05
17	0	1025	CLA	CHC-C1C	2.16	1.42	1.37
17	P	8009	CLA	C1B-CHB	-2.16	1.33	1.40
17	B	1240	CLA	CHC-C1C	2.16	1.42	1.37
17	Q	5242	CLA	CHC-C1C	2.16	1.42	1.37
17	8	1012	CLA	CHC-C1C	2.15	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5235	CLA	C1D-CHD	2.16	1.42	1.36
17	4	4002	CLA	C1B-CHB	-2.15	1.33	1.40
17	Q	5223	CLA	C1C-NC	-2.15	1.36	1.39
17	B	1213	CLA	C1D-CHD	2.15	1.42	1.36
17	0	1015	CLA	C1B-CHB	-2.15	1.33	1.40
17	Q	5213	CLA	C1D-CHD	2.15	1.42	1.36
17	4	4002	CLA	CHC-C1C	2.15	1.42	1.37
17	B	1215	CLA	C1C-NC	-2.15	1.36	1.39
17	8	1017	CLA	CHC-C1C	2.15	1.42	1.37
17	B	1209	CLA	C1C-NC	-2.15	1.36	1.39
17	4	1023	CLA	CHC-C1C	2.15	1.42	1.37
17	0	1031	CLA	C1B-CHB	-2.15	1.33	1.40
17	V	5701	CLA	C1B-CHB	-2.15	1.33	1.40
17	Z	8008	CLA	CHC-C1C	2.15	1.42	1.37
17	8	1025	CLA	CHC-C1C	2.15	1.42	1.37
17	A	1113	CLA	CHC-C1C	2.15	1.42	1.37
17	0	1015	CLA	CHC-C1C	2.15	1.42	1.37
17	P	5107	CLA	C1D-CHD	2.15	1.42	1.36
17	P	5117	CLA	C1D-CHD	2.15	1.42	1.36
17	3	1016	CLA	CHC-C1C	2.15	1.42	1.37
17	1	1017	CLA	CHC-C1C	2.15	1.42	1.37
17	P	5113	CLA	CHC-C1C	2.15	1.42	1.37
17	1	1023	CLA	CHC-C1C	2.15	1.42	1.37
17	3	1011	CLA	CHC-C1C	2.15	1.42	1.37
17	8	1014	CLA	CHC-C1C	2.15	1.42	1.37
17	L	1504	CLA	CHC-C1C	2.15	1.42	1.37
17	P	5115	CLA	C1B-CHB	-2.15	1.33	1.40
17	8	1022	CLA	CHC-C1C	2.15	1.42	1.37
17	B	1230	CLA	C1D-CHD	2.15	1.42	1.36
17	A	4009	CLA	C1B-CHB	-2.15	1.33	1.40
17	7	1012	CLA	C1B-CHB	-2.14	1.33	1.40
17	3	1017	CLA	C1B-CHB	-2.14	1.33	1.40
17	2	1015	CLA	C1B-CHB	-2.14	1.33	1.40
17	2	1015	CLA	CHC-C1C	2.15	1.42	1.37
17	0	1017	CLA	CHC-C1C	2.14	1.42	1.37
17	U	8005	CLA	CHC-C1C	2.14	1.42	1.37
17	7	1021	CLA	CHC-C1C	2.14	1.42	1.37
17	4	1017	CLA	CHC-C1C	2.14	1.42	1.37
17	J	4008	CLA	CHC-C1C	2.14	1.42	1.37
17	A	1117	CLA	C1D-CHD	2.14	1.42	1.36
17	G	1233	CLA	CHC-C1C	2.14	1.42	1.37
17	A	1106	CLA	C1B-CHB	-2.14	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	1021	CLA	CHC-C1C	2.14	1.42	1.37
17	8	1025	CLA	C1B-CHB	-2.14	1.33	1.40
17	4	1015	CLA	C1B-CHB	-2.14	1.33	1.40
17	1	1016	CLA	C1B-CHB	-2.14	1.33	1.40
17	7	1023	CLA	CHC-C1C	2.14	1.42	1.37
17	8	1011	CLA	C1B-CHB	-2.14	1.33	1.40
17	Q	5230	CLA	C1D-CHD	2.14	1.42	1.36
17	P	5106	CLA	C1B-CHB	-2.14	1.33	1.40
17	Q	5221	CLA	C1B-CHB	-2.14	1.33	1.40
17	Q	5240	CLA	CHC-C1C	2.14	1.42	1.37
17	Q	5236	CLA	C1B-CHB	-2.14	1.33	1.40
17	9	1041	CLA	C1B-CHB	-2.14	1.33	1.40
17	9	1017	CLA	CHC-C1C	2.14	1.42	1.37
17	A	1133	CLA	MG-NB	2.14	2.09	2.05
17	3	1022	CLA	CHC-C1C	2.14	1.42	1.37
17	P	8009	CLA	CHC-C1C	2.14	1.42	1.37
17	F	4005	CLA	CHC-C1C	2.14	1.42	1.37
17	H	1801	CLA	CHC-C1C	2.14	1.42	1.37
17	3	1014	CLA	C1B-CHB	-2.14	1.33	1.40
17	2	1025	CLA	C1B-CHB	-2.14	1.33	1.40
17	9	1032	CLA	C1B-CHB	-2.14	1.33	1.40
17	2	1011	CLA	C1B-CHB	-2.14	1.33	1.40
17	1	1026	CLA	C1B-CHB	-2.14	1.33	1.40
17	2	4007	CLA	CHC-C1C	2.14	1.42	1.37
17	3	1033	CLA	CHC-C1C	2.14	1.42	1.37
17	Q	8001	CLA	C1B-CHB	-2.14	1.33	1.40
17	B	1223	CLA	C1C-NC	-2.14	1.36	1.39
17	A	1115	CLA	C1B-CHB	-2.14	1.33	1.40
17	8	1013	CLA	CHC-C1C	2.14	1.42	1.37
17	P	8010	CLA	CHC-C1C	2.14	1.42	1.37
17	U	8004	CLA	CHC-C1C	2.14	1.42	1.37
17	P	5112	CLA	C1B-CHB	-2.14	1.33	1.40
17	6	5504	CLA	CHC-C1C	2.14	1.42	1.37
17	G	1233	CLA	C1C-NC	-2.14	1.36	1.39
17	5	5403	CLA	CHC-C1C	2.14	1.42	1.37
17	0	1021	CLA	CHC-C1C	2.14	1.42	1.37
17	9	1033	CLA	CHC-C1C	2.14	1.42	1.37
17	0	1013	CLA	C1B-CHB	-2.14	1.33	1.40
17	B	4001	CLA	C1B-CHB	-2.14	1.33	1.40
17	G	1701	CLA	C1B-CHB	-2.14	1.33	1.40
17	G	1701	CLA	CHC-C1C	2.14	1.42	1.37
17	2	1026	CLA	CHC-C1C	2.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	5701	CLA	CHC-C1C	2.14	1.42	1.37
17	8	1031	CLA	C1B-CHB	-2.14	1.33	1.40
17	3	1041	CLA	C1B-CHB	-2.14	1.33	1.40
17	B	1236	CLA	C1B-CHB	-2.14	1.33	1.40
17	P	5110	CLA	C1C-NC	-2.14	1.36	1.39
17	3	1015	CLA	CHC-C1C	2.13	1.42	1.37
17	4	1015	CLA	CHC-C1C	2.13	1.42	1.37
17	3	1031	CLA	CHC-C1C	2.13	1.42	1.37
17	2	1031	CLA	C1B-CHB	-2.13	1.33	1.40
17	A	1107	CLA	C1D-CHD	2.13	1.42	1.36
17	A	4010	CLA	CHC-C1C	2.13	1.42	1.37
17	8	1026	CLA	CHC-C1C	2.13	1.42	1.37
17	U	5229	CLA	C1D-CHD	2.13	1.42	1.36
17	2	1016	CLA	CHC-C1C	2.13	1.42	1.37
17	Q	5023	CLA	C1C-NC	-2.13	1.36	1.39
17	2	1017	CLA	CHC-C1C	2.13	1.42	1.37
17	7	1016	CLA	C1B-CHB	-2.13	1.33	1.40
17	7	1031	CLA	CHC-C1C	2.13	1.42	1.37
17	A	4009	CLA	CHC-C1C	2.13	1.42	1.37
17	8	1015	CLA	C1B-CHB	-2.13	1.33	1.40
17	1	1025	CLA	C1B-CHB	-2.13	1.33	1.40
17	0	1016	CLA	C1B-CHB	-2.13	1.33	1.40
17	J	4008	CLA	C1B-CHB	-2.13	1.33	1.40
17	B	1241	CLA	C1B-CHB	-2.13	1.33	1.40
17	Q	5240	CLA	C1B-CHB	-2.13	1.33	1.40
17	8	1026	CLA	C1B-CHB	-2.13	1.33	1.40
17	3	1041	CLA	CHC-C1C	2.13	1.42	1.37
17	1	1031	CLA	CHC-C1C	2.13	1.42	1.37
17	2	1033	CLA	C1B-CHB	-2.13	1.33	1.40
17	B	1235	CLA	C1B-CHB	-2.13	1.33	1.40
17	2	1023	CLA	CHC-C1C	2.13	1.42	1.37
17	3	1012	CLA	CHC-C1C	2.13	1.42	1.37
17	4	1031	CLA	C1B-CHB	-2.13	1.33	1.40
17	0	1025	CLA	C1B-CHB	-2.13	1.33	1.40
17	Q	5235	CLA	C1B-CHB	-2.13	1.33	1.40
17	A	1011	CLA	CHC-C1C	2.13	1.42	1.37
17	2	1012	CLA	CHC-C1C	2.13	1.42	1.37
17	Q	5205	CLA	CHC-C1C	2.13	1.42	1.37
17	2	1026	CLA	C1B-CHB	-2.13	1.33	1.40
17	4	1025	CLA	C1B-CHB	-2.13	1.33	1.40
17	P	8010	CLA	C1B-CHB	-2.13	1.33	1.40
17	P	5011	CLA	CHC-C1C	2.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	1012	CLA	CHC-C1C	2.13	1.42	1.37
17	7	1013	CLA	CHC-C1C	2.13	1.42	1.37
17	3	1032	CLA	C1B-CHB	-2.13	1.33	1.40
17	2	1025	CLA	CHC-C1C	2.13	1.42	1.37
17	9	1011	CLA	CHC-C1C	2.13	1.42	1.37
17	V	5233	CLA	CHC-C1C	2.13	1.42	1.37
17	B	1210	CLA	C1B-CHB	-2.13	1.33	1.40
17	1	1012	CLA	CHC-C1C	2.13	1.42	1.37
17	4	1026	CLA	C1B-CHB	-2.13	1.33	1.40
17	3	1021	CLA	C1B-CHB	-2.13	1.33	1.40
17	8	1033	CLA	C1B-CHB	-2.13	1.33	1.40
17	3	1026	CLA	C1B-CHB	-2.13	1.33	1.40
17	4	1033	CLA	C1B-CHB	-2.13	1.33	1.40
17	4	1017	CLA	C1B-CHB	-2.13	1.33	1.40
17	4	1016	CLA	C1B-CHB	-2.13	1.33	1.40
17	4	1011	CLA	C1B-CHB	-2.13	1.33	1.40
17	F	4003	CLA	CHC-C1C	2.13	1.42	1.37
17	Z	8008	CLA	C1B-CHB	-2.13	1.33	1.40
17	A	4010	CLA	C1B-CHB	-2.13	1.33	1.40
17	0	1014	CLA	C1B-CHB	-2.13	1.33	1.40
17	J	1101	CLA	CHC-C1C	2.13	1.42	1.37
17	8	1017	CLA	C1B-CHB	-2.13	1.33	1.40
17	2	1012	CLA	C1B-CHB	-2.13	1.33	1.40
17	5	5404	CLA	C1B-CHB	-2.13	1.33	1.40
17	9	1031	CLA	CHC-C1C	2.12	1.42	1.37
17	U	8003	CLA	C1B-CHB	-2.12	1.33	1.40
17	W	5801	CLA	CHC-C1C	2.12	1.42	1.37
17	B	1240	CLA	C1B-CHB	-2.13	1.33	1.40
17	7	1025	CLA	C1B-CHB	-2.12	1.33	1.40
17	8	1023	CLA	C1B-CHB	-2.12	1.33	1.40
17	9	1022	CLA	CHC-C1C	2.12	1.42	1.37
17	A	1112	CLA	C1B-CHB	-2.12	1.33	1.40
17	7	1022	CLA	CHC-C1C	2.12	1.42	1.37
17	0	1033	CLA	C1B-CHB	-2.12	1.33	1.40
17	Z	5101	CLA	CHC-C1C	2.12	1.42	1.37
17	7	1011	CLA	CHC-C1C	2.12	1.42	1.37
17	9	1026	CLA	C1B-CHB	-2.12	1.33	1.40
17	9	1014	CLA	C1B-CHB	-2.12	1.33	1.40
17	F	4003	CLA	C1B-CHB	-2.12	1.33	1.40
17	9	1021	CLA	C1B-CHB	-2.12	1.33	1.40
17	3	1017	CLA	CHC-C1C	2.12	1.42	1.37
17	8	1016	CLA	CHC-C1C	2.12	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	U	8004	CLA	C1B-CHB	-2.12	1.33	1.40
17	7	1026	CLA	C1B-CHB	-2.12	1.33	1.40
17	K	1404	CLA	C1B-CHB	-2.12	1.33	1.40
17	8	8007	CLA	C1D-CHD	2.12	1.42	1.36
17	Q	5212	CLA	C1C-NC	-2.12	1.36	1.39
17	F	4004	CLA	C1B-CHB	-2.12	1.33	1.40
17	F	4004	CLA	CHC-C1C	2.12	1.42	1.37
17	U	8005	CLA	C1B-CHB	-2.12	1.33	1.40
17	Q	5210	CLA	C1B-CHB	-2.12	1.33	1.40
17	9	1031	CLA	C1B-CHB	-2.12	1.33	1.40
17	L	1504	CLA	C1B-CHB	-2.12	1.33	1.40
17	4	1022	CLA	C1B-CHB	-2.12	1.33	1.40
17	Q	5241	CLA	C1B-CHB	-2.12	1.33	1.40
17	3	1022	CLA	C1B-CHB	-2.12	1.33	1.40
17	U	8003	CLA	CHC-C1C	2.12	1.42	1.37
17	2	1017	CLA	C1B-CHB	-2.12	1.33	1.40
17	9	1022	CLA	C1B-CHB	-2.12	1.33	1.40
17	Q	8001	CLA	CHC-C1C	2.12	1.42	1.37
17	U	8006	CLA	C1B-CHB	-2.12	1.33	1.40
17	4	1014	CLA	CHC-C1C	2.12	1.42	1.37
17	F	4006	CLA	C1B-CHB	-2.12	1.33	1.40
17	2	1023	CLA	C1B-CHB	-2.12	1.33	1.40
17	0	1026	CLA	CHC-C1C	2.12	1.42	1.37
17	K	1403	CLA	CHC-C1C	2.12	1.42	1.37
17	2	1015	CLA	C1D-CHD	2.12	1.42	1.36
17	K	1404	CLA	CHC-C1C	2.12	1.42	1.37
17	8	8007	CLA	CHC-C1C	2.12	1.42	1.37
17	8	1023	CLA	CHC-C1C	2.12	1.42	1.37
17	J	1101	CLA	C1B-CHB	-2.12	1.33	1.40
17	B	1205	CLA	CHC-C1C	2.12	1.42	1.37
17	F	1229	CLA	C1D-CHD	2.12	1.42	1.36
17	2	1021	CLA	CHC-C1C	2.12	1.42	1.37
17	7	1023	CLA	C1B-CHB	-2.12	1.33	1.40
17	1	1013	CLA	CHC-C1C	2.12	1.42	1.37
17	B	4001	CLA	CHC-C1C	2.12	1.42	1.37
17	4	1014	CLA	C1B-CHB	-2.11	1.33	1.40
17	1	1012	CLA	C1B-CHB	-2.11	1.33	1.40
17	1	1023	CLA	C1B-CHB	-2.11	1.33	1.40
17	0	1022	CLA	C1B-CHB	-2.11	1.33	1.40
17	8	1021	CLA	CHC-C1C	2.11	1.42	1.37
17	1	1011	CLA	CHC-C1C	2.11	1.42	1.37
17	4	1013	CLA	C1B-CHB	-2.11	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	1015	CLA	CHC-C1C	2.11	1.42	1.37
17	H	1801	CLA	C1B-CHB	-2.11	1.33	1.40
17	Q	5230	CLA	CHC-C1C	2.11	1.42	1.37
17	1	1022	CLA	C1B-CHB	-2.11	1.33	1.40
17	W	5801	CLA	C1B-CHB	-2.11	1.33	1.40
17	0	1026	CLA	C1B-CHB	-2.11	1.33	1.40
17	0	1011	CLA	C1B-CHB	-2.11	1.33	1.40
17	F	4005	CLA	C1B-CHB	-2.11	1.33	1.40
17	7	1016	CLA	CHC-C1C	2.11	1.42	1.37
17	9	1025	CLA	C1B-CHB	-2.11	1.33	1.40
17	0	1012	CLA	CHC-C1C	2.11	1.42	1.37
17	1	1022	CLA	CHC-C1C	2.11	1.42	1.37
17	2	1013	CLA	C1B-CHB	-2.11	1.33	1.40
17	2	1013	CLA	CHC-C1C	2.11	1.42	1.37
17	A	1116	CLA	MG-NC	2.11	2.13	2.07
17	8	1015	CLA	C1D-CHD	2.11	1.42	1.36
17	Q	5241	CLA	C1D-CHD	2.11	1.42	1.36
17	4	1021	CLA	C1B-CHB	-2.11	1.33	1.40
17	1	1021	CLA	C1B-CHB	-2.11	1.33	1.40
17	B	1230	CLA	CHC-C1C	2.11	1.42	1.37
17	7	1012	CLA	CHC-C1C	2.11	1.42	1.37
17	1	1011	CLA	C1B-CHB	-2.11	1.33	1.40
17	A	1133	CLA	CHC-C1C	2.11	1.42	1.37
17	8	1017	CLA	C1D-CHD	2.11	1.42	1.36
17	0	1033	CLA	CHC-C1C	2.11	1.42	1.37
17	3	1032	CLA	CHC-C1C	2.11	1.42	1.37
17	4	1021	CLA	CHC-C1C	2.11	1.42	1.37
17	4	1012	CLA	CHC-C1C	2.11	1.42	1.37
17	B	1242	CLA	C1B-CHB	-2.11	1.33	1.40
17	4	1033	CLA	CHC-C1C	2.11	1.42	1.37
17	5	5404	CLA	CHC-C1C	2.11	1.42	1.37
17	A	1121	CLA	CHC-C1C	2.11	1.42	1.37
17	7	1017	CLA	C1B-CHB	-2.11	1.33	1.40
17	0	1017	CLA	C1B-CHB	-2.11	1.33	1.40
17	2	4007	CLA	C1D-CHD	2.11	1.42	1.36
17	2	1016	CLA	C1B-CHB	-2.11	1.33	1.40
17	4	1026	CLA	CHC-C1C	2.11	1.42	1.37
17	7	1021	CLA	C1B-CHB	-2.11	1.33	1.40
17	B	1241	CLA	C1D-CHD	2.11	1.42	1.36
17	0	1016	CLA	CHC-C1C	2.11	1.42	1.37
17	8	1022	CLA	C1B-CHB	-2.11	1.33	1.40
17	7	1026	CLA	C1D-CHD	2.11	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	1013	CLA	C1B-CHB	-2.10	1.33	1.40
17	0	1013	CLA	CHC-C1C	2.11	1.42	1.37
17	P	5116	CLA	MG-NC	2.11	2.13	2.07
17	0	1031	CLA	CHC-C1C	2.10	1.42	1.37
17	2	1026	CLA	C1D-CHD	2.10	1.42	1.36
17	1	1013	CLA	C1B-CHB	-2.10	1.33	1.40
17	4	1023	CLA	C1B-CHB	-2.10	1.33	1.40
17	1	1014	CLA	C1B-CHB	-2.10	1.33	1.40
17	V	5701	CLA	C1D-CHD	2.10	1.42	1.36
17	1	1016	CLA	CHC-C1C	2.10	1.42	1.37
17	9	1016	CLA	C1B-CHB	-2.10	1.33	1.40
17	8	1012	CLA	C1B-CHB	-2.10	1.33	1.40
17	3	1031	CLA	C1B-CHB	-2.10	1.33	1.40
17	1	1025	CLA	CHC-C1C	2.10	1.42	1.37
17	1	1015	CLA	CHC-C1C	2.10	1.42	1.37
17	7	1022	CLA	C1B-CHB	-2.10	1.33	1.40
17	9	1032	CLA	CHC-C1C	2.10	1.42	1.37
17	G	1701	CLA	C1D-CHD	2.10	1.42	1.36
17	4	1032	CLA	C1B-CHB	-2.10	1.33	1.40
17	3	1016	CLA	C1B-CHB	-2.10	1.33	1.40
17	2	1014	CLA	C1B-CHB	-2.10	1.33	1.40
17	4	1013	CLA	CHC-C1C	2.10	1.42	1.37
17	A	4009	CLA	C1D-CHD	2.10	1.42	1.36
17	3	1025	CLA	C1B-CHB	-2.10	1.33	1.40
17	6	5504	CLA	C1B-CHB	-2.10	1.33	1.40
17	7	1025	CLA	CHC-C1C	2.10	1.42	1.37
17	3	1015	CLA	C1B-CHB	-2.10	1.33	1.40
17	3	1033	CLA	C1B-CHB	-2.10	1.33	1.40
17	9	1041	CLA	C1D-CHD	2.10	1.42	1.36
17	1	1031	CLA	C1B-CHB	-2.10	1.33	1.40
17	0	1021	CLA	C1B-CHB	-2.10	1.33	1.40
17	2	1021	CLA	C1B-CHB	-2.10	1.33	1.40
17	K	1403	CLA	C1B-CHB	-2.10	1.33	1.40
17	0	1032	CLA	CHC-C1C	2.10	1.42	1.37
17	B	1212	CLA	C1C-NC	-2.10	1.36	1.39
17	4	1016	CLA	CHC-C1C	2.10	1.42	1.37
17	4	1016	CLA	C1D-CHD	2.10	1.42	1.36
17	0	1025	CLA	C1D-CHD	2.10	1.42	1.36
17	8	1013	CLA	C1B-CHB	-2.10	1.33	1.40
17	1	1017	CLA	C1B-CHB	-2.10	1.33	1.40
17	0	1023	CLA	C1B-CHB	-2.10	1.33	1.40
17	0	1033	CLA	C1D-CHD	2.10	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	P	6001	PQN	C8-C7	2.10	1.44	1.37
17	V	5233	CLA	C1C-NC	-2.10	1.36	1.39
17	Z	5101	CLA	C1B-CHB	-2.10	1.33	1.40
17	7	1011	CLA	C1B-CHB	-2.09	1.33	1.40
17	Q	5242	CLA	C1B-CHB	-2.10	1.33	1.40
17	8	1021	CLA	C1B-CHB	-2.10	1.33	1.40
17	3	1012	CLA	C1D-CHD	2.10	1.42	1.36
17	9	1015	CLA	CHC-C1C	2.10	1.42	1.37
17	8	1012	CLA	C1D-CHD	2.10	1.42	1.36
17	4	1031	CLA	CHC-C1C	2.10	1.42	1.37
17	7	1025	CLA	C1D-CHD	2.10	1.42	1.36
17	8	1016	CLA	C1B-CHB	-2.10	1.33	1.40
17	A	1131	CLA	MG-NC	2.09	2.13	2.07
17	8	1026	CLA	C1D-CHD	2.10	1.42	1.36
17	2	1012	CLA	C1D-CHD	2.10	1.42	1.36
17	P	5112	CLA	C1C-NC	-2.09	1.36	1.39
17	9	1033	CLA	C1B-CHB	-2.09	1.33	1.40
17	U	8006	CLA	C1D-CHD	2.09	1.42	1.36
17	2	1022	CLA	C1B-CHB	-2.09	1.33	1.40
17	P	5121	CLA	CHC-C1C	2.09	1.42	1.37
17	8	8007	CLA	C1B-CHB	-2.09	1.33	1.40
17	B	1023	CLA	C1C-NC	-2.09	1.36	1.39
17	1	1015	CLA	C1B-CHB	-2.09	1.33	1.40
17	6	5504	CLA	C1D-CHD	2.09	1.42	1.36
17	8	1023	CLA	C1D-CHD	2.09	1.42	1.36
17	8	1011	CLA	CHC-C1C	2.09	1.42	1.37
17	4	1026	CLA	C1D-CHD	2.09	1.42	1.36
17	7	1014	CLA	C1B-CHB	-2.09	1.33	1.40
17	5	5403	CLA	C1B-CHB	-2.09	1.33	1.40
17	3	1012	CLA	C1B-CHB	-2.09	1.33	1.40
17	9	1015	CLA	C1B-CHB	-2.09	1.33	1.40
17	0	1026	CLA	C1D-CHD	2.09	1.42	1.36
18	A	2001	PQN	C8-C7	2.09	1.43	1.37
17	0	1012	CLA	C1D-CHD	2.09	1.42	1.36
17	9	1032	CLA	C1D-CHD	2.09	1.42	1.36
17	3	1026	CLA	CHC-C1C	2.09	1.42	1.37
17	4	1033	CLA	C1D-CHD	2.09	1.42	1.36
17	0	1014	CLA	CHC-C1C	2.09	1.42	1.37
17	2	1023	CLA	C1D-CHD	2.08	1.42	1.36
17	B	1223	CLA	MG-NC	2.08	2.13	2.07
17	9	1021	CLA	C1D-CHD	2.09	1.42	1.36
17	Q	5240	CLA	C1D-CHD	2.09	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	1012	CLA	C1B-CHB	-2.08	1.33	1.40
17	7	1031	CLA	C1D-CHD	2.08	1.42	1.36
17	2	1011	CLA	CHC-C1C	2.08	1.42	1.37
17	A	1103	CLA	C1B-CHB	-2.08	1.33	1.40
17	3	1033	CLA	C1D-CHD	2.08	1.42	1.36
18	Q	6002	PQN	C10-C1	-2.08	1.44	1.48
17	W	5801	CLA	C1D-CHD	2.08	1.42	1.36
17	B	1227	CLA	C1B-CHB	-2.08	1.33	1.40
17	4	1032	CLA	CHC-C1C	2.08	1.42	1.37
17	P	5131	CLA	MG-NC	2.08	2.13	2.07
17	8	1014	CLA	C1B-CHB	-2.08	1.33	1.40
17	3	1014	CLA	C1D-CHD	2.08	1.42	1.36
17	Q	5223	CLA	MG-NC	2.08	2.13	2.07
17	0	1031	CLA	C1D-CHD	2.08	1.42	1.36
17	8	1013	CLA	C1D-CHD	2.08	1.42	1.36
17	4	1031	CLA	C1D-CHD	2.08	1.42	1.36
17	3	1022	CLA	C1D-CHD	2.08	1.42	1.36
17	P	5133	CLA	CHC-C1C	2.08	1.42	1.37
17	1	1026	CLA	C1D-CHD	2.08	1.42	1.36
17	A	1013	CLA	CHC-C1C	2.08	1.42	1.37
17	8	1025	CLA	C1D-CHD	2.08	1.42	1.36
17	4	1012	CLA	C1D-CHD	2.08	1.42	1.36
17	0	1032	CLA	C1B-CHB	-2.08	1.33	1.40
17	P	5103	CLA	C1B-CHB	-2.08	1.33	1.40
17	9	1012	CLA	C1D-CHD	2.08	1.42	1.36
17	A	1112	CLA	C1C-NC	-2.08	1.36	1.39
17	7	1031	CLA	C1B-CHB	-2.08	1.33	1.40
17	9	1016	CLA	C1D-CHD	2.08	1.42	1.36
17	1	1025	CLA	C1D-CHD	2.08	1.42	1.36
17	L	1504	CLA	C1D-CHD	2.08	1.42	1.36
17	8	1021	CLA	C1D-CHD	2.07	1.42	1.36
17	P	5111	CLA	CHC-C1C	2.08	1.42	1.37
17	H	1801	CLA	C1D-CHD	2.08	1.42	1.36
17	1	1015	CLA	C1D-CHD	2.07	1.42	1.36
17	3	1041	CLA	C1D-CHD	2.08	1.42	1.36
17	5	5404	CLA	C1D-CHD	2.08	1.42	1.36
17	9	1026	CLA	CHC-C1C	2.07	1.42	1.37
17	2	1022	CLA	C1D-CHD	2.07	1.42	1.36
17	4	1025	CLA	C1D-CHD	2.07	1.42	1.36
17	F	4006	CLA	C1D-CHD	2.07	1.42	1.36
17	3	1015	CLA	C1D-CHD	2.07	1.42	1.36
17	2	4007	CLA	C1B-CHB	-2.07	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	0	1016	CLA	C1D-CHD	2.07	1.42	1.36
17	2	1017	CLA	C1D-CHD	2.07	1.42	1.36
17	9	1022	CLA	C1D-CHD	2.07	1.42	1.36
17	7	1015	CLA	C1B-CHB	-2.07	1.33	1.40
17	K	1404	CLA	C1D-CHD	2.07	1.42	1.36
17	P	8009	CLA	C1D-CHD	2.07	1.42	1.36
17	1	1031	CLA	C1D-CHD	2.07	1.42	1.36
17	7	1011	CLA	C1D-CHD	2.07	1.42	1.36
17	1	1016	CLA	C1D-CHD	2.07	1.42	1.36
19	R	7002	SF4	S1-FE4	-2.07	2.31	2.33
17	0	1023	CLA	C1D-CHD	2.07	1.42	1.36
17	1	1014	CLA	CHC-C1C	2.07	1.42	1.37
17	A	1111	CLA	CHC-C1C	2.07	1.42	1.37
17	4	1023	CLA	C1D-CHD	2.07	1.42	1.36
17	0	8002	CLA	C1D-CHD	2.07	1.42	1.36
17	1	1023	CLA	C1D-CHD	2.07	1.42	1.36
17	4	1014	CLA	C1D-CHD	2.07	1.42	1.36
17	9	1015	CLA	C1D-CHD	2.07	1.42	1.36
17	3	1031	CLA	C1D-CHD	2.07	1.42	1.36
17	4	1032	CLA	C1D-CHD	2.07	1.42	1.36
17	8	1033	CLA	C1D-CHD	2.07	1.42	1.36
17	0	1011	CLA	C1D-CHD	2.07	1.42	1.36
17	J	4008	CLA	C1D-CHD	2.07	1.42	1.36
17	0	1014	CLA	C1D-CHD	2.07	1.42	1.36
17	4	1011	CLA	C1D-CHD	2.07	1.42	1.36
17	8	1011	CLA	C1D-CHD	2.07	1.42	1.36
17	B	1240	CLA	C1D-CHD	2.07	1.42	1.36
17	F	4004	CLA	C1D-CHD	2.07	1.42	1.36
17	Q	8001	CLA	C1D-CHD	2.07	1.42	1.36
17	1	1011	CLA	C1D-CHD	2.07	1.42	1.36
17	P	5136	CLA	C1B-CHB	-2.07	1.34	1.40
17	3	1026	CLA	C1D-CHD	2.07	1.42	1.36
17	J	1101	CLA	C1D-CHD	2.07	1.42	1.36
17	B	1232	CLA	C1B-CHB	-2.06	1.34	1.40
17	3	1021	CLA	C1D-CHD	2.07	1.42	1.36
17	Q	5216	CLA	C1D-CHD	2.07	1.42	1.36
17	9	1031	CLA	C1D-CHD	2.06	1.42	1.36
17	B	1231	CLA	C1B-CHB	-2.06	1.34	1.40
17	F	4005	CLA	C1D-CHD	2.06	1.42	1.36
17	Q	5212	CLA	MG-NC	2.06	2.13	2.07
17	Q	5232	CLA	C1B-CHB	-2.06	1.34	1.40
17	3	1032	CLA	C1D-CHD	2.06	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	1025	CLA	C1D-CHD	2.06	1.42	1.36
17	2	1013	CLA	C1D-CHD	2.06	1.42	1.36
17	A	1132	CLA	C1B-CHB	-2.06	1.34	1.40
17	7	1016	CLA	C1D-CHD	2.06	1.42	1.36
17	Q	5227	CLA	C1B-CHB	-2.06	1.34	1.40
17	4	1017	CLA	C1D-CHD	2.06	1.42	1.36
17	7	1013	CLA	C1D-CHD	2.06	1.42	1.36
17	8	1022	CLA	C1D-CHD	2.06	1.42	1.36
17	7	1017	CLA	C1D-CHD	2.06	1.42	1.36
17	K	1403	CLA	C1D-CHD	2.06	1.42	1.36
17	7	1015	CLA	C1D-CHD	2.06	1.42	1.36
17	0	1021	CLA	C1D-CHD	2.06	1.42	1.36
17	U	8005	CLA	C1D-CHD	2.06	1.42	1.36
17	0	1015	CLA	C1D-CHD	2.06	1.42	1.36
17	7	1023	CLA	C1D-CHD	2.06	1.42	1.36
17	3	1011	CLA	C1D-CHD	2.06	1.42	1.36
17	B	1216	CLA	C1D-CHD	2.06	1.42	1.36
17	F	4003	CLA	C1D-CHD	2.06	1.42	1.36
17	P	5114	CLA	CHC-C1C	2.06	1.42	1.37
17	1	1013	CLA	C1D-CHD	2.06	1.42	1.36
17	Z	5101	CLA	C1D-CHD	2.06	1.42	1.36
17	2	1021	CLA	C1D-CHD	2.05	1.42	1.36
17	0	1032	CLA	C1D-CHD	2.06	1.42	1.36
17	3	1016	CLA	C1D-CHD	2.06	1.42	1.36
17	U	8003	CLA	C1D-CHD	2.06	1.42	1.36
17	Q	5232	CLA	C1D-CHD	2.06	1.42	1.36
17	P	8010	CLA	C1D-CHD	2.06	1.42	1.36
17	B	1242	CLA	C1D-CHD	2.05	1.42	1.36
17	A	4010	CLA	C1D-CHD	2.05	1.42	1.36
17	1	1014	CLA	C1D-CHD	2.05	1.42	1.36
17	4	1022	CLA	C1D-CHD	2.05	1.42	1.36
17	3	1017	CLA	C1D-CHD	2.05	1.42	1.36
17	A	1114	CLA	CHC-C1C	2.05	1.42	1.37
17	7	1012	CLA	C1D-CHD	2.05	1.42	1.36
17	Q	5219	CLA	C1D-CHD	2.05	1.42	1.36
17	B	4001	CLA	C1D-CHD	2.05	1.42	1.36
17	2	1031	CLA	C1D-CHD	2.05	1.42	1.36
18	B	2002	PQN	C10-C1	-2.05	1.44	1.48
17	B	1227	CLA	C1C-NC	-2.05	1.36	1.39
17	2	1033	CLA	C1D-CHD	2.05	1.42	1.36
17	A	1136	CLA	C1B-CHB	-2.05	1.34	1.40
17	Q	5242	CLA	C1D-CHD	2.05	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	1033	CLA	C1D-CHD	2.05	1.42	1.36
17	Z	8008	CLA	C1D-CHD	2.05	1.42	1.36
17	9	1026	CLA	C1D-CHD	2.05	1.42	1.36
17	Q	5130	CLA	MG-NC	2.05	2.13	2.07
17	P	5132	CLA	C1B-CHB	-2.05	1.34	1.40
17	Q	5231	CLA	C1B-CHB	-2.05	1.34	1.40
17	B	1212	CLA	MG-NC	2.05	2.13	2.07
17	4	4002	CLA	C1D-CHD	2.05	1.42	1.36
17	8	1031	CLA	C1D-CHD	2.05	1.42	1.36
17	2	1011	CLA	C1D-CHD	2.05	1.42	1.36
17	U	8004	CLA	C1D-CHD	2.05	1.42	1.36
17	P	5013	CLA	CHC-C1C	2.05	1.42	1.37
17	9	1014	CLA	C1D-CHD	2.05	1.42	1.36
17	B	1219	CLA	C1D-CHD	2.05	1.42	1.36
17	B	1130	CLA	MG-NC	2.05	2.13	2.07
17	1	1012	CLA	C1D-CHD	2.04	1.42	1.36
17	1	1017	CLA	C1D-CHD	2.05	1.42	1.36
17	8	1016	CLA	C1D-CHD	2.05	1.42	1.36
17	4	1015	CLA	C1D-CHD	2.04	1.42	1.36
17	A	1114	CLA	C1D-CHD	2.04	1.42	1.36
17	0	1017	CLA	C1D-CHD	2.04	1.42	1.36
17	P	5109	CLA	CHC-C1C	2.04	1.42	1.37
17	7	1021	CLA	C1D-CHD	2.04	1.42	1.36
17	5	5403	CLA	C1D-CHD	2.04	1.42	1.36
17	4	1021	CLA	C1D-CHD	2.04	1.42	1.36
17	P	5122	CLA	C1B-CHB	-2.04	1.34	1.40
17	7	1014	CLA	CHC-C1C	2.04	1.42	1.37
17	P	5125	CLA	C1D-CHD	2.04	1.42	1.36
17	0	1022	CLA	C1D-CHD	2.04	1.42	1.36
17	B	1216	CLA	MG-NC	2.04	2.13	2.07
17	Q	5211	CLA	C1B-CHB	-2.04	1.34	1.40
17	9	1011	CLA	C1D-CHD	2.04	1.42	1.36
17	1	1021	CLA	C1D-CHD	2.03	1.42	1.36
17	P	5111	CLA	C1B-CHB	-2.03	1.34	1.40
17	9	1017	CLA	C1D-CHD	2.03	1.42	1.36
17	P	5114	CLA	C1D-CHD	2.03	1.42	1.36
17	7	1014	CLA	C1D-CHD	2.03	1.42	1.36
17	6	5501	CLA	C1D-CHD	2.03	1.42	1.36
17	2	1016	CLA	C1D-CHD	2.03	1.42	1.36
17	8	1014	CLA	C1D-CHD	2.03	1.42	1.36
17	A	1111	CLA	C1B-CHB	-2.03	1.34	1.40
17	A	1125	CLA	C1D-CHD	2.03	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1109	CLA	CHC-C1C	2.03	1.42	1.37
17	B	1232	CLA	C1D-CHD	2.03	1.42	1.36
17	Q	5216	CLA	C1B-CHB	-2.03	1.34	1.40
17	2	1014	CLA	C1D-CHD	2.03	1.41	1.36
17	A	1127	CLA	C1C-NC	-2.03	1.36	1.39
17	7	1022	CLA	C1D-CHD	2.02	1.41	1.36
17	A	1122	CLA	C1B-CHB	-2.02	1.34	1.40
17	A	1129	CLA	C1C-NC	-2.02	1.36	1.39
17	B	1216	CLA	C1B-CHB	-2.02	1.34	1.40
17	P	5121	CLA	MG-NC	2.02	2.13	2.07
17	1	1022	CLA	C1D-CHD	2.02	1.41	1.36
17	B	1211	CLA	C1B-CHB	-2.02	1.34	1.40
17	Q	5216	CLA	MG-NC	2.02	2.13	2.07
17	K	1401	CLA	C1B-CHB	-2.01	1.34	1.40
17	A	1108	CLA	C1D-CHD	2.01	1.41	1.36
17	0	8002	CLA	C1C-NC	-2.01	1.36	1.39
17	4	4002	CLA	C1C-NC	-2.01	1.36	1.39
17	A	1121	CLA	MG-NC	2.01	2.13	2.07
17	Q	5222	CLA	CHC-C1C	2.01	1.42	1.37
17	L	1503	CLA	C1D-CHD	2.01	1.41	1.36
17	P	5103	CLA	C1D-CHD	2.01	1.41	1.36
17	A	1109	CLA	C1B-CHB	-2.01	1.34	1.40
17	P	5109	CLA	C1B-CHB	-2.01	1.34	1.40
17	A	1137	CLA	C1D-CHD	2.01	1.41	1.36
17	7	1011	CLA	C1C-NC	-2.01	1.36	1.39
17	3	1025	CLA	C1D-CHD	2.01	1.41	1.36
17	B	1226	CLA	C1C-NC	-2.01	1.36	1.39
17	L	1501	CLA	C1D-CHD	2.01	1.41	1.36
18	B	2002	PQN	C8-C7	2.01	1.43	1.37
17	Q	5227	CLA	C1C-NC	-2.01	1.36	1.39
19	C	3002	SF4	S1-FE4	-2.01	2.31	2.33
17	P	5119	CLA	C1C-NC	-2.01	1.36	1.39
17	A	1103	CLA	C1D-CHD	2.00	1.41	1.36
17	A	1116	CLA	C1D-CHD	2.00	1.41	1.36
17	1	1011	CLA	C1C-NC	-2.00	1.36	1.39
18	P	6001	PQN	C8-C9	2.00	1.43	1.39
17	P	5137	CLA	C1D-CHD	2.00	1.41	1.36
17	8	1015	CLA	C1C-NC	-2.00	1.36	1.39
17	B	1214	CLA	C1D-CHD	2.00	1.41	1.36
17	5	5401	CLA	C1B-CHB	-2.00	1.34	1.40
17	8	1012	CLA	C1C-NC	-2.00	1.36	1.39
17	P	5126	CLA	C1B-CHB	-2.00	1.34	1.40

All (702) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Z	5302	CLA	C4A-NA-C1A	6.10	114.24	106.22
17	J	1302	CLA	C4A-NA-C1A	6.09	114.22	106.22
17	A	1901	CLA	C4A-NA-C1A	5.96	114.05	106.22
17	P	5901	CLA	C4A-NA-C1A	5.95	114.03	106.22
17	A	1113	CLA	C4A-NA-C1A	5.67	113.67	106.22
17	P	5113	CLA	C4A-NA-C1A	5.64	113.63	106.22
17	B	1219	CLA	C4A-NA-C1A	5.55	113.52	106.22
17	Q	5219	CLA	C4A-NA-C1A	5.52	113.47	106.22
17	A	1108	CLA	C4A-NA-C1A	5.07	112.89	106.22
17	P	5103	CLA	C4A-NA-C1A	5.07	112.88	106.22
17	A	1103	CLA	C4A-NA-C1A	5.06	112.86	106.22
17	P	5108	CLA	C4A-NA-C1A	5.05	112.85	106.22
17	P	5137	CLA	C4A-NA-C1A	4.91	112.67	106.22
17	A	1137	CLA	C4A-NA-C1A	4.90	112.66	106.22
17	A	1135	CLA	C4A-NA-C1A	4.85	112.60	106.22
17	P	5111	CLA	C4A-NA-C1A	4.85	112.59	106.22
17	A	1111	CLA	C4A-NA-C1A	4.85	112.59	106.22
17	P	5135	CLA	C4A-NA-C1A	4.81	112.54	106.22
17	Q	5130	CLA	C4A-NA-C1A	4.81	112.53	106.22
17	Q	5204	CLA	C4A-NA-C1A	4.78	112.50	106.22
17	B	1204	CLA	C4A-NA-C1A	4.78	112.50	106.22
17	B	1130	CLA	C4A-NA-C1A	4.77	112.49	106.22
17	A	1402	CLA	C4A-NA-C1A	4.75	112.46	106.22
17	Q	5223	CLA	C4A-NA-C1A	4.73	112.43	106.22
17	B	1223	CLA	C4A-NA-C1A	4.72	112.43	106.22
17	P	5123	CLA	C4A-NA-C1A	4.72	112.43	106.22
17	P	5402	CLA	C4A-NA-C1A	4.71	112.41	106.22
17	A	1123	CLA	C4A-NA-C1A	4.71	112.41	106.22
17	B	1202	CLA	C4A-NA-C1A	4.69	112.38	106.22
17	Q	5202	CLA	C4A-NA-C1A	4.69	112.38	106.22
17	B	1239	CLA	C4A-NA-C1A	4.65	112.33	106.22
17	Q	5239	CLA	C4A-NA-C1A	4.64	112.32	106.22
17	A	1125	CLA	C4A-NA-C1A	4.63	112.31	106.22
17	P	5125	CLA	C4A-NA-C1A	4.62	112.29	106.22
17	P	5110	CLA	C4A-NA-C1A	4.61	112.28	106.22
17	B	1206	CLA	C4A-NA-C1A	4.60	112.26	106.22
17	Q	5206	CLA	C4A-NA-C1A	4.59	112.25	106.22
17	A	1110	CLA	C4A-NA-C1A	4.58	112.24	106.22
17	O	8002	CLA	C4A-NA-C1A	4.58	112.23	106.22
17	Q	5207	CLA	C4A-NA-C1A	4.58	112.23	106.22
17	B	1221	CLA	C4A-NA-C1A	4.58	112.23	106.22
17	Q	5221	CLA	C4A-NA-C1A	4.57	112.23	106.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	1207	CLA	C4A-NA-C1A	4.55	112.19	106.22
17	4	4002	CLA	C4A-NA-C1A	4.54	112.19	106.22
17	0	1032	CLA	C4A-NA-C1A	4.53	112.17	106.22
17	2	1016	CLA	C4A-NA-C1A	4.52	112.16	106.22
17	1	1022	CLA	C4A-NA-C1A	4.52	112.16	106.22
17	5	5404	CLA	C4A-NA-C1A	4.52	112.16	106.22
17	8	1016	CLA	C4A-NA-C1A	4.52	112.16	106.22
17	B	1217	CLA	C4A-NA-C1A	4.52	112.16	106.22
17	3	1032	CLA	C4A-NA-C1A	4.52	112.16	106.22
17	9	1033	CLA	C4A-NA-C1A	4.52	112.15	106.22
17	8	1014	CLA	C4A-NA-C1A	4.52	112.15	106.22
17	0	1022	CLA	C4A-NA-C1A	4.51	112.15	106.22
17	9	1012	CLA	C4A-NA-C1A	4.51	112.14	106.22
17	4	1022	CLA	C4A-NA-C1A	4.51	112.14	106.22
17	7	1011	CLA	C4A-NA-C1A	4.51	112.14	106.22
17	3	1022	CLA	C4A-NA-C1A	4.50	112.14	106.22
17	8	1026	CLA	C4A-NA-C1A	4.51	112.14	106.22
17	1	1011	CLA	C4A-NA-C1A	4.50	112.13	106.22
17	U	8005	CLA	C4A-NA-C1A	4.50	112.13	106.22
17	4	1031	CLA	C4A-NA-C1A	4.50	112.13	106.22
17	9	1032	CLA	C4A-NA-C1A	4.50	112.13	106.22
17	7	1015	CLA	C4A-NA-C1A	4.50	112.13	106.22
17	B	1210	CLA	C4A-NA-C1A	4.50	112.13	106.22
17	Q	5210	CLA	C4A-NA-C1A	4.50	112.13	106.22
17	4	1032	CLA	C4A-NA-C1A	4.50	112.13	106.22
17	2	1014	CLA	C4A-NA-C1A	4.50	112.13	106.22
17	7	1017	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	0	1015	CLA	C4A-NA-C1A	4.49	112.13	106.22
17	Q	5217	CLA	C4A-NA-C1A	4.50	112.13	106.22
17	3	1012	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	Z	5101	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	2	1026	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	8	1013	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	3	1025	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	8	1022	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	F	4005	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	7	1026	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	1	1015	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	7	1022	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	2	1011	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	2	1022	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	K	1404	CLA	C4A-NA-C1A	4.49	112.11	106.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	9	1025	CLA	C4A-NA-C1A	4.49	112.11	106.22
17	9	1011	CLA	C4A-NA-C1A	4.49	112.12	106.22
17	3	1033	CLA	C4A-NA-C1A	4.49	112.11	106.22
17	4	1015	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	2	1031	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	F	4003	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	3	1026	CLA	C4A-NA-C1A	4.49	112.11	106.22
17	Q	5241	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	9	1022	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	8	1031	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	B	1231	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	0	1031	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	0	1011	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	4	1011	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	F	4004	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	1	1031	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	J	4008	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	G	1701	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	Z	8008	CLA	C4A-NA-C1A	4.48	112.11	106.22
17	H	1801	CLA	C4A-NA-C1A	4.48	112.10	106.22
17	3	1014	CLA	C4A-NA-C1A	4.48	112.10	106.22
17	9	1014	CLA	C4A-NA-C1A	4.48	112.10	106.22
17	1	1025	CLA	C4A-NA-C1A	4.48	112.10	106.22
17	F	4006	CLA	C4A-NA-C1A	4.47	112.10	106.22
17	3	1015	CLA	C4A-NA-C1A	4.48	112.10	106.22
17	U	8006	CLA	C4A-NA-C1A	4.48	112.10	106.22
17	A	4009	CLA	C4A-NA-C1A	4.48	112.10	106.22
17	8	8007	CLA	C4A-NA-C1A	4.47	112.10	106.22
17	1	1026	CLA	C4A-NA-C1A	4.47	112.10	106.22
17	9	1026	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	3	1011	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	8	1012	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	4	1033	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	7	1025	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	J	1101	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	P	8010	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	1	1017	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	4	1016	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	2	1013	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	3	1041	CLA	C4A-NA-C1A	4.47	112.09	106.22
17	1	1021	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	5	5403	CLA	C4A-NA-C1A	4.46	112.09	106.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	0	1033	CLA	C4A-NA-C1A	4.46	112.09	106.22
17	4	1017	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	8	1011	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	W	5801	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	4	1026	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	K	1403	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	V	5701	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	9	1021	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	1	1014	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	B	1240	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	6	5504	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	8	1023	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	3	1017	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	7	1031	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	2	4007	CLA	C4A-NA-C1A	4.46	112.08	106.22
17	2	1023	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	B	1242	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	3	1031	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	L	1504	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	0	1016	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	8	1017	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	2	1015	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	P	8009	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	B	4001	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	1	1012	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	7	1021	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	U	8004	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	2	1017	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	1	1013	CLA	C4A-NA-C1A	4.45	112.07	106.22
17	7	1012	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	4	1013	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	A	4010	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	7	1013	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	2	1012	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	Q	5242	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	3	1021	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	9	1015	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	Q	5231	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	9	1031	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	4	1023	CLA	C4A-NA-C1A	4.45	112.06	106.22
17	U	8003	CLA	C4A-NA-C1A	4.44	112.06	106.22
17	Q	8001	CLA	C4A-NA-C1A	4.44	112.06	106.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	1016	CLA	C4A-NA-C1A	4.44	112.06	106.22
17	9	1017	CLA	C4A-NA-C1A	4.44	112.06	106.22
17	B	1234	CLA	C4A-NA-C1A	4.44	112.06	106.22
17	0	1017	CLA	C4A-NA-C1A	4.44	112.06	106.22
17	0	1026	CLA	C4A-NA-C1A	4.44	112.06	106.22
17	7	1016	CLA	C4A-NA-C1A	4.44	112.06	106.22
17	4	1014	CLA	C4A-NA-C1A	4.44	112.05	106.22
17	9	1041	CLA	C4A-NA-C1A	4.44	112.05	106.22
17	A	1118	CLA	C4A-NA-C1A	4.44	112.05	106.22
17	4	1012	CLA	C4A-NA-C1A	4.44	112.05	106.22
17	P	5140	CLA	C4A-NA-C1A	4.44	112.05	106.22
17	B	1241	CLA	C4A-NA-C1A	4.44	112.05	106.22
17	0	1023	CLA	C4A-NA-C1A	4.44	112.05	106.22
17	A	1140	CLA	C4A-NA-C1A	4.44	112.05	106.22
17	B	1224	CLA	C4A-NA-C1A	4.44	112.05	106.22
17	2	1025	CLA	C4A-NA-C1A	4.44	112.05	106.22
17	1	1023	CLA	C4A-NA-C1A	4.43	112.05	106.22
17	8	1025	CLA	C4A-NA-C1A	4.43	112.04	106.22
17	8	1015	CLA	C4A-NA-C1A	4.43	112.04	106.22
17	Q	5234	CLA	C4A-NA-C1A	4.43	112.04	106.22
17	A	1104	CLA	C4A-NA-C1A	4.43	112.04	106.22
17	P	5118	CLA	C4A-NA-C1A	4.43	112.04	106.22
17	3	1016	CLA	C4A-NA-C1A	4.42	112.03	106.22
17	G	1233	CLA	C4A-NA-C1A	4.42	112.03	106.22
17	7	1023	CLA	C4A-NA-C1A	4.42	112.03	106.22
17	P	5012	CLA	C4A-NA-C1A	4.42	112.03	106.22
17	7	1014	CLA	C4A-NA-C1A	4.42	112.03	106.22
17	4	1025	CLA	C4A-NA-C1A	4.42	112.03	106.22
17	Q	5240	CLA	C4A-NA-C1A	4.42	112.03	106.22
17	B	1021	CLA	C4A-NA-C1A	4.42	112.02	106.22
17	0	1013	CLA	C4A-NA-C1A	4.42	112.03	106.22
17	0	1012	CLA	C4A-NA-C1A	4.42	112.03	106.22
17	Q	5224	CLA	C4A-NA-C1A	4.42	112.02	106.22
17	0	1021	CLA	C4A-NA-C1A	4.41	112.02	106.22
17	9	1016	CLA	C4A-NA-C1A	4.41	112.02	106.22
17	4	1021	CLA	C4A-NA-C1A	4.41	112.02	106.22
17	P	5104	CLA	C4A-NA-C1A	4.41	112.01	106.22
17	8	1033	CLA	C4A-NA-C1A	4.41	112.01	106.22
17	0	1014	CLA	C4A-NA-C1A	4.41	112.01	106.22
17	2	1033	CLA	C4A-NA-C1A	4.40	112.00	106.22
17	A	1012	CLA	C4A-NA-C1A	4.40	112.01	106.22
17	8	1021	CLA	C4A-NA-C1A	4.40	112.01	106.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	5021	CLA	C4A-NA-C1A	4.40	112.00	106.22
17	V	5233	CLA	C4A-NA-C1A	4.39	111.99	106.22
17	O	1025	CLA	C4A-NA-C1A	4.39	111.99	106.22
17	2	1021	CLA	C4A-NA-C1A	4.39	111.99	106.22
17	P	5134	CLA	C4A-NA-C1A	4.38	111.97	106.22
17	A	1134	CLA	C4A-NA-C1A	4.38	111.97	106.22
17	Q	5209	CLA	C4A-NA-C1A	4.37	111.97	106.22
17	A	1129	CLA	C4A-NA-C1A	4.37	111.96	106.22
17	F	1301	CLA	C4A-NA-C1A	4.37	111.96	106.22
17	U	5301	CLA	C4A-NA-C1A	4.37	111.96	106.22
17	Q	5203	CLA	C4A-NA-C1A	4.37	111.96	106.22
17	B	1209	CLA	C4A-NA-C1A	4.37	111.96	106.22
17	A	1114	CLA	C4A-NA-C1A	4.37	111.96	106.22
17	P	5114	CLA	C4A-NA-C1A	4.36	111.95	106.22
17	P	5129	CLA	C4A-NA-C1A	4.36	111.95	106.22
17	B	1203	CLA	C4A-NA-C1A	4.35	111.94	106.22
17	B	1218	CLA	C4A-NA-C1A	4.35	111.94	106.22
17	P	5131	CLA	C4A-NA-C1A	4.34	111.92	106.22
17	A	1131	CLA	C4A-NA-C1A	4.32	111.90	106.22
17	A	1107	CLA	C4A-NA-C1A	4.32	111.90	106.22
17	Q	5218	CLA	C4A-NA-C1A	4.32	111.89	106.22
17	P	5107	CLA	C4A-NA-C1A	4.32	111.89	106.22
17	Q	5214	CLA	C4A-NA-C1A	4.31	111.88	106.22
17	Q	5212	CLA	C4A-NA-C1A	4.31	111.88	106.22
17	Q	5228	CLA	C4A-NA-C1A	4.31	111.88	106.22
17	A	1133	CLA	C4A-NA-C1A	4.30	111.87	106.22
17	B	1212	CLA	C4A-NA-C1A	4.29	111.86	106.22
17	B	1214	CLA	C4A-NA-C1A	4.29	111.85	106.22
17	B	1228	CLA	C4A-NA-C1A	4.28	111.84	106.22
17	P	5133	CLA	C4A-NA-C1A	4.28	111.84	106.22
17	Q	5201	CLA	C4A-NA-C1A	4.28	111.84	106.22
17	B	1201	CLA	C4A-NA-C1A	4.26	111.82	106.22
17	P	5106	CLA	C4A-NA-C1A	4.26	111.82	106.22
17	P	5124	CLA	C4A-NA-C1A	4.26	111.82	106.22
17	P	5137	CLA	C1C-NC-C4C	4.26	111.83	106.28
17	A	1106	CLA	C4A-NA-C1A	4.26	111.81	106.22
17	P	5127	CLA	C4A-NA-C1A	4.25	111.80	106.22
17	A	1102	CLA	C4A-NA-C1A	4.24	111.80	106.22
17	A	1137	CLA	C1C-NC-C4C	4.24	111.81	106.28
17	B	1222	CLA	C4A-NA-C1A	4.23	111.78	106.22
17	A	1124	CLA	C4A-NA-C1A	4.23	111.77	106.22
17	P	5102	CLA	C4A-NA-C1A	4.22	111.77	106.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	5109	CLA	C4A-NA-C1A	4.22	111.76	106.22
17	A	1127	CLA	C4A-NA-C1A	4.22	111.76	106.22
17	Q	5222	CLA	C4A-NA-C1A	4.21	111.76	106.22
17	U	5229	CLA	C4A-NA-C1A	4.20	111.74	106.22
17	Q	5235	CLA	C4A-NA-C1A	4.20	111.74	106.22
17	P	5138	CLA	C4A-NA-C1A	4.20	111.74	106.22
17	P	5122	CLA	C4A-NA-C1A	4.20	111.73	106.22
17	A	1138	CLA	C4A-NA-C1A	4.20	111.73	106.22
17	Q	5215	CLA	C4A-NA-C1A	4.20	111.74	106.22
17	A	1122	CLA	C4A-NA-C1A	4.20	111.74	106.22
17	B	1235	CLA	C4A-NA-C1A	4.19	111.73	106.22
17	Q	5211	CLA	C4A-NA-C1A	4.19	111.73	106.22
17	A	1120	CLA	C4A-NA-C1A	4.19	111.72	106.22
17	B	1211	CLA	C4A-NA-C1A	4.19	111.72	106.22
17	A	1109	CLA	C4A-NA-C1A	4.18	111.71	106.22
17	Q	5230	CLA	C4A-NA-C1A	4.18	111.71	106.22
17	F	1229	CLA	C4A-NA-C1A	4.18	111.71	106.22
17	B	1230	CLA	C4A-NA-C1A	4.17	111.70	106.22
17	Q	5237	CLA	C4A-NA-C1A	4.17	111.70	106.22
17	B	1215	CLA	C4A-NA-C1A	4.17	111.70	106.22
17	P	5120	CLA	C4A-NA-C1A	4.16	111.69	106.22
17	Q	5227	CLA	C4A-NA-C1A	4.16	111.69	106.22
17	B	1227	CLA	C4A-NA-C1A	4.16	111.69	106.22
17	B	1237	CLA	C4A-NA-C1A	4.15	111.68	106.22
17	Q	5236	CLA	C4A-NA-C1A	4.14	111.66	106.22
17	A	1116	CLA	C4A-NA-C1A	4.13	111.65	106.22
17	A	1901	CLA	C1C-NC-C4C	4.12	111.66	106.28
17	P	5116	CLA	C4A-NA-C1A	4.12	111.64	106.22
17	B	1236	CLA	C4A-NA-C1A	4.11	111.62	106.22
17	P	5139	CLA	C4A-NA-C1A	4.11	111.62	106.22
17	6	5502	CLA	C4A-NA-C1A	4.11	111.62	106.22
17	A	1139	CLA	C4A-NA-C1A	4.10	111.61	106.22
17	P	5117	CLA	C4A-NA-C1A	4.08	111.58	106.22
17	A	1117	CLA	C4A-NA-C1A	4.08	111.58	106.22
17	A	1105	CLA	C4A-NA-C1A	4.08	111.58	106.22
17	P	5901	CLA	C1C-NC-C4C	4.08	111.60	106.28
17	P	5132	CLA	C4A-NA-C1A	4.08	111.58	106.22
17	A	1132	CLA	C4A-NA-C1A	4.08	111.58	106.22
17	A	1011	CLA	C4A-NA-C1A	4.08	111.58	106.22
17	P	5011	CLA	C4A-NA-C1A	4.08	111.58	106.22
17	P	5105	CLA	C4A-NA-C1A	4.07	111.57	106.22
17	L	1502	CLA	C4A-NA-C1A	4.07	111.56	106.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	1401	CLA	C4A-NA-C1A	4.06	111.55	106.22
17	5	5401	CLA	C4A-NA-C1A	4.05	111.54	106.22
17	A	1119	CLA	C4A-NA-C1A	4.04	111.53	106.22
17	Q	5216	CLA	C4A-NA-C1A	4.04	111.53	106.22
17	B	1216	CLA	C4A-NA-C1A	4.04	111.53	106.22
17	Q	5220	CLA	C4A-NA-C1A	4.04	111.52	106.22
17	P	5119	CLA	C4A-NA-C1A	4.03	111.51	106.22
17	P	5113	CLA	C1C-NC-C4C	4.03	111.53	106.28
17	B	1220	CLA	C4A-NA-C1A	4.02	111.50	106.22
17	B	1232	CLA	C4A-NA-C1A	4.01	111.49	106.22
17	A	1113	CLA	C1C-NC-C4C	4.01	111.51	106.28
17	B	1208	CLA	C4A-NA-C1A	4.01	111.48	106.22
17	B	1022	CLA	C4A-NA-C1A	4.00	111.48	106.22
17	Q	5232	CLA	C4A-NA-C1A	4.01	111.48	106.22
17	Q	5022	CLA	C4A-NA-C1A	4.00	111.47	106.22
17	A	1126	CLA	C4A-NA-C1A	4.00	111.47	106.22
17	P	5126	CLA	C4A-NA-C1A	4.00	111.47	106.22
17	Q	5208	CLA	C4A-NA-C1A	3.99	111.46	106.22
17	Q	5023	CLA	C4A-NA-C1A	3.98	111.46	106.22
17	B	1023	CLA	C4A-NA-C1A	3.99	111.46	106.22
17	A	1112	CLA	C4A-NA-C1A	3.97	111.44	106.22
17	Q	5238	CLA	C4A-NA-C1A	3.97	111.44	106.22
17	B	1238	CLA	C4A-NA-C1A	3.97	111.44	106.22
17	L	1503	CLA	C4A-NA-C1A	3.95	111.41	106.22
17	6	5503	CLA	C4A-NA-C1A	3.95	111.41	106.22
17	P	5112	CLA	C4A-NA-C1A	3.95	111.41	106.22
17	B	1213	CLA	C4A-NA-C1A	3.87	111.31	106.22
17	Q	5213	CLA	C4A-NA-C1A	3.87	111.31	106.22
17	Q	5205	CLA	C4A-NA-C1A	3.87	111.30	106.22
17	B	1205	CLA	C4A-NA-C1A	3.87	111.30	106.22
17	J	1302	CLA	C4B-NB-C1B	3.86	111.84	106.76
17	A	1013	CLA	C4A-NA-C1A	3.85	111.28	106.22
17	P	5121	CLA	C4A-NA-C1A	3.84	111.27	106.22
17	Z	5302	CLA	C4B-NB-C1B	3.84	111.82	106.76
17	A	1121	CLA	C4A-NA-C1A	3.82	111.24	106.22
17	P	5013	CLA	C4A-NA-C1A	3.81	111.23	106.22
17	P	5136	CLA	C4A-NA-C1A	3.80	111.21	106.22
17	A	1136	CLA	C4A-NA-C1A	3.79	111.20	106.22
17	Q	5219	CLA	C1C-NC-C4C	3.77	111.20	106.28
17	A	1108	CLA	C1C-NC-C4C	3.77	111.20	106.28
17	P	5108	CLA	C1C-NC-C4C	3.76	111.19	106.28
17	B	1219	CLA	C1C-NC-C4C	3.76	111.19	106.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	5501	CLA	C4A-NA-C1A	3.76	111.16	106.22
17	P	5115	CLA	C4A-NA-C1A	3.73	111.12	106.22
17	L	1501	CLA	C4A-NA-C1A	3.73	111.12	106.22
17	A	1115	CLA	C4A-NA-C1A	3.72	111.11	106.22
17	Q	5226	CLA	C4A-NA-C1A	3.71	111.10	106.22
17	P	5128	CLA	C4A-NA-C1A	3.70	111.08	106.22
17	B	1226	CLA	C4A-NA-C1A	3.69	111.07	106.22
17	A	1128	CLA	C4A-NA-C1A	3.67	111.04	106.22
17	A	1901	CLA	CHD-C4C-NC	3.67	127.44	124.49
17	P	5901	CLA	CHD-C4C-NC	3.59	127.37	124.49
17	Z	5302	CLA	C1C-NC-C4C	3.50	110.85	106.28
17	J	1302	CLA	C1C-NC-C4C	3.49	110.83	106.28
17	A	1113	CLA	C4B-NB-C1B	3.45	111.31	106.76
17	P	5113	CLA	C4B-NB-C1B	3.45	111.31	106.76
17	Q	5225	CLA	C4A-NA-C1A	3.45	110.75	106.22
17	B	1225	CLA	C4A-NA-C1A	3.43	110.72	106.22
17	P	5108	CLA	C4B-NB-C1B	3.10	110.84	106.76
17	B	1219	CLA	C4B-NB-C1B	3.08	110.83	106.76
17	A	1108	CLA	C4B-NB-C1B	3.08	110.82	106.76
17	Q	5219	CLA	C4B-NB-C1B	3.06	110.79	106.76
17	A	1901	CLA	C4B-NB-C1B	2.98	110.68	106.76
17	P	5901	CLA	C4B-NB-C1B	2.97	110.67	106.76
17	Q	5223	CLA	C4B-NB-C1B	2.95	110.65	106.76
17	B	1022	CLA	C1C-NC-C4C	2.95	110.13	106.28
17	B	1223	CLA	C4B-NB-C1B	2.95	110.65	106.76
17	Q	5022	CLA	C1C-NC-C4C	2.95	110.12	106.28
17	Q	5023	CLA	C1C-NC-C4C	2.92	110.09	106.28
17	P	5137	CLA	C4B-NB-C1B	2.88	110.56	106.76
17	B	1023	CLA	C1C-NC-C4C	2.87	110.03	106.28
17	A	1137	CLA	C4B-NB-C1B	2.85	110.51	106.76
17	A	1137	CLA	CHD-C4C-NC	2.83	126.76	124.49
17	P	5137	CLA	CHD-C4C-NC	2.81	126.75	124.49
17	P	5118	CLA	C1C-NC-C4C	2.79	109.92	106.28
17	A	1118	CLA	C1C-NC-C4C	2.79	109.91	106.28
17	P	5125	CLA	C4B-NB-C1B	2.77	110.42	106.76
17	A	1125	CLA	C4B-NB-C1B	2.76	110.40	106.76
17	P	5113	CLA	CHD-C4C-NC	2.74	126.69	124.49
17	Q	5207	CLA	C4B-NB-C1B	2.72	110.34	106.76
17	A	1126	CLA	C1C-NC-C4C	2.71	109.82	106.28
17	P	5126	CLA	C1C-NC-C4C	2.71	109.82	106.28
17	A	1116	CLA	C1C-NC-C4C	2.70	109.81	106.28
17	A	1113	CLA	CHD-C4C-NC	2.71	126.66	124.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	5116	CLA	C1C-NC-C4C	2.69	109.80	106.28
17	B	1207	CLA	C4B-NB-C1B	2.69	110.31	106.76
17	Q	5219	CLA	CHD-C4C-NC	2.67	126.64	124.49
17	B	1219	CLA	CHD-C4C-NC	2.65	126.62	124.49
17	B	1204	CLA	C1C-NC-C4C	2.63	109.71	106.28
17	Q	5204	CLA	C1C-NC-C4C	2.62	109.70	106.28
17	B	1231	CLA	C1C-NC-C4C	2.62	109.70	106.28
17	B	1235	CLA	C1C-NC-C4C	2.59	109.66	106.28
17	Q	5235	CLA	C1C-NC-C4C	2.59	109.66	106.28
17	6	5502	CLA	C1C-NC-C4C	2.58	109.64	106.28
17	4	1012	CLA	C4B-NB-C1B	2.57	110.15	106.76
17	P	5119	CLA	C1C-NC-C4C	2.57	109.64	106.28
17	Q	5231	CLA	C1C-NC-C4C	2.57	109.63	106.28
17	P	5129	CLA	C1C-NC-C4C	2.56	109.62	106.28
17	Q	5221	CLA	C4B-NB-C1B	2.56	110.14	106.76
17	Q	5227	CLA	C1C-NC-C4C	2.56	109.62	106.28
17	0	1031	CLA	C4B-NB-C1B	2.56	110.14	106.76
17	B	1228	CLA	C1C-NC-C4C	2.56	109.62	106.28
17	9	1014	CLA	C4B-NB-C1B	2.56	110.13	106.76
17	B	1227	CLA	C1C-NC-C4C	2.56	109.62	106.28
17	A	1129	CLA	C1C-NC-C4C	2.56	109.62	106.28
17	Q	5228	CLA	C1C-NC-C4C	2.56	109.62	106.28
17	A	1119	CLA	C1C-NC-C4C	2.55	109.61	106.28
17	4	1031	CLA	C4B-NB-C1B	2.55	110.12	106.76
17	Q	5202	CLA	C4B-NB-C1B	2.55	110.12	106.76
17	Q	5220	CLA	C1C-NC-C4C	2.55	109.60	106.28
17	8	8007	CLA	C4B-NB-C1B	2.54	110.11	106.76
17	B	1221	CLA	C4B-NB-C1B	2.54	110.11	106.76
17	7	1025	CLA	C4B-NB-C1B	2.54	110.11	106.76
17	0	1012	CLA	C4B-NB-C1B	2.54	110.11	106.76
17	5	5404	CLA	C4B-NB-C1B	2.54	110.11	106.76
17	0	1022	CLA	C4B-NB-C1B	2.54	110.11	106.76
17	B	1202	CLA	C4B-NB-C1B	2.54	110.11	106.76
17	9	1011	CLA	C4B-NB-C1B	2.54	110.11	106.76
17	8	1033	CLA	C4B-NB-C1B	2.54	110.11	106.76
17	L	1502	CLA	C1C-NC-C4C	2.53	109.59	106.28
17	3	1014	CLA	C4B-NB-C1B	2.53	110.10	106.76
17	0	1011	CLA	C4B-NB-C1B	2.53	110.10	106.76
17	7	1013	CLA	C4B-NB-C1B	2.53	110.10	106.76
17	9	1012	CLA	C4B-NB-C1B	2.53	110.10	106.76
17	4	1011	CLA	C4B-NB-C1B	2.53	110.10	106.76
17	Q	5241	CLA	C4B-NB-C1B	2.53	110.10	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	4007	CLA	C4B-NB-C1B	2.53	110.09	106.76
17	9	1026	CLA	C4B-NB-C1B	2.53	110.09	106.76
17	8	1012	CLA	C4B-NB-C1B	2.53	110.09	106.76
17	1	1025	CLA	C4B-NB-C1B	2.53	110.09	106.76
17	4	1022	CLA	C4B-NB-C1B	2.53	110.09	106.76
17	8	1011	CLA	C4B-NB-C1B	2.53	110.09	106.76
17	3	1012	CLA	C4B-NB-C1B	2.53	110.09	106.76
17	K	1403	CLA	C4B-NB-C1B	2.52	110.09	106.76
17	0	1015	CLA	C4B-NB-C1B	2.52	110.09	106.76
17	3	1033	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	B	1210	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	K	1404	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	Q	8001	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	4	1026	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	2	1017	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	B	1220	CLA	C1C-NC-C4C	2.52	109.57	106.28
17	9	1033	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	3	1011	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	3	1026	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	4	1015	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	9	1022	CLA	C4B-NB-C1B	2.51	110.08	106.76
17	2	1012	CLA	C4B-NB-C1B	2.52	110.08	106.76
17	1	1023	CLA	C4B-NB-C1B	2.51	110.07	106.76
17	7	1011	CLA	C4B-NB-C1B	2.51	110.07	106.76
17	7	1023	CLA	C4B-NB-C1B	2.51	110.07	106.76
17	0	1026	CLA	C4B-NB-C1B	2.51	110.07	106.76
17	P	5402	CLA	C4B-NB-C1B	2.51	110.07	106.76
17	9	1017	CLA	C4B-NB-C1B	2.51	110.07	106.76
17	P	8010	CLA	C4B-NB-C1B	2.51	110.07	106.76
17	3	1032	CLA	C4B-NB-C1B	2.51	110.07	106.76
17	Q	5210	CLA	C4B-NB-C1B	2.51	110.07	106.76
17	8	1017	CLA	C4B-NB-C1B	2.51	110.07	106.76
17	9	1032	CLA	C4B-NB-C1B	2.51	110.06	106.76
17	1	1011	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	9	1031	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	7	1026	CLA	C4B-NB-C1B	2.51	110.06	106.76
17	2	1011	CLA	C4B-NB-C1B	2.51	110.06	106.76
17	A	4010	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	1	1022	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	1	1026	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	0	8002	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	4	1025	CLA	C4B-NB-C1B	2.50	110.06	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	1033	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	B	1241	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	0	1025	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	4	4002	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	5	5403	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	8	1025	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	W	5801	CLA	C4B-NB-C1B	2.50	110.06	106.76
17	G	1701	CLA	C4B-NB-C1B	2.50	110.05	106.76
17	V	5701	CLA	C4B-NB-C1B	2.50	110.05	106.76
17	L	1504	CLA	C4B-NB-C1B	2.50	110.05	106.76
17	F	4003	CLA	C4B-NB-C1B	2.50	110.05	106.76
17	7	1022	CLA	C4B-NB-C1B	2.50	110.05	106.76
17	2	1025	CLA	C4B-NB-C1B	2.50	110.05	106.76
17	1	1013	CLA	C4B-NB-C1B	2.50	110.05	106.76
17	B	4001	CLA	C4B-NB-C1B	2.50	110.05	106.76
17	B	1215	CLA	C1C-NC-C4C	2.50	109.54	106.28
17	Q	5215	CLA	C1C-NC-C4C	2.49	109.54	106.28
17	2	1033	CLA	C4B-NB-C1B	2.49	110.05	106.76
17	3	1022	CLA	C4B-NB-C1B	2.49	110.05	106.76
17	0	1033	CLA	C4B-NB-C1B	2.49	110.05	106.76
17	7	1015	CLA	C4B-NB-C1B	2.49	110.05	106.76
17	4	1023	CLA	C4B-NB-C1B	2.49	110.05	106.76
17	3	1041	CLA	C4B-NB-C1B	2.49	110.04	106.76
17	B	1226	CLA	C4B-NB-C1B	2.49	110.04	106.76
17	3	1017	CLA	C4B-NB-C1B	2.49	110.04	106.76
17	J	1101	CLA	C4B-NB-C1B	2.49	110.04	106.76
17	7	1016	CLA	C4B-NB-C1B	2.49	110.04	106.76
17	A	4009	CLA	C4B-NB-C1B	2.49	110.04	106.76
17	U	8004	CLA	C4B-NB-C1B	2.48	110.04	106.76
17	1	1017	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	7	1031	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	8	1013	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	6	5504	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	0	1014	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	1	1014	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	B	1242	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	7	1017	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	0	1016	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	2	1026	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	3	1031	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	U	8003	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	2	1013	CLA	C4B-NB-C1B	2.48	110.02	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	9	1041	CLA	C4B-NB-C1B	2.48	110.02	106.76
17	8	1015	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	Q	5203	CLA	C4B-NB-C1B	2.48	110.03	106.76
17	A	1108	CLA	CHD-C4C-NC	2.48	126.48	124.49
17	0	1023	CLA	C4B-NB-C1B	2.48	110.02	106.76
17	4	1014	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	H	1801	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	4	1016	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	3	1015	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	7	1012	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	U	8005	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	8	1023	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	Q	5226	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	J	4008	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	A	1402	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	P	8009	CLA	C4B-NB-C1B	2.47	110.02	106.76
17	Q	5242	CLA	C4B-NB-C1B	2.47	110.01	106.76
17	4	1013	CLA	C4B-NB-C1B	2.47	110.01	106.76
17	Q	5240	CLA	C4B-NB-C1B	2.47	110.01	106.76
17	0	1013	CLA	C4B-NB-C1B	2.47	110.01	106.76
17	8	1022	CLA	C4B-NB-C1B	2.47	110.01	106.76
17	4	1021	CLA	C4B-NB-C1B	2.47	110.01	106.76
17	F	4006	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	Z	5101	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	F	4004	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	1	1031	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	0	1021	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	1	1016	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	1	1015	CLA	C4B-NB-C1B	2.47	110.01	106.76
17	8	1016	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	1	1012	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	3	1021	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	2	1015	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	B	1240	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	2	1022	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	3	1025	CLA	C4B-NB-C1B	2.46	110.01	106.76
17	8	1021	CLA	C4B-NB-C1B	2.46	110.00	106.76
17	P	5108	CLA	CHD-C4C-NC	2.46	126.47	124.49
17	9	1015	CLA	C4B-NB-C1B	2.46	110.00	106.76
17	2	1021	CLA	C4B-NB-C1B	2.46	110.00	106.76
17	8	1026	CLA	C4B-NB-C1B	2.46	110.00	106.76
17	2	1016	CLA	C4B-NB-C1B	2.45	110.00	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	1023	CLA	C4B-NB-C1B	2.46	110.00	106.76
17	F	4005	CLA	C4B-NB-C1B	2.45	110.00	106.76
17	Z	8008	CLA	C4B-NB-C1B	2.45	110.00	106.76
17	7	1021	CLA	C4B-NB-C1B	2.45	109.99	106.76
17	0	1017	CLA	C4B-NB-C1B	2.45	109.99	106.76
17	4	1017	CLA	C4B-NB-C1B	2.45	109.99	106.76
17	3	1016	CLA	C4B-NB-C1B	2.45	109.99	106.76
17	9	1025	CLA	C4B-NB-C1B	2.45	109.99	106.76
17	U	8006	CLA	C4B-NB-C1B	2.45	109.98	106.76
17	Q	5237	CLA	C1C-NC-C4C	2.45	109.47	106.28
17	4	1032	CLA	C4B-NB-C1B	2.45	109.98	106.76
17	U	5229	CLA	C1C-NC-C4C	2.45	109.47	106.28
17	0	1032	CLA	C4B-NB-C1B	2.44	109.98	106.76
17	P	5123	CLA	C4B-NB-C1B	2.44	109.98	106.76
17	1	1021	CLA	C4B-NB-C1B	2.44	109.98	106.76
17	B	1203	CLA	C4B-NB-C1B	2.44	109.97	106.76
17	2	1031	CLA	C4B-NB-C1B	2.44	109.97	106.76
17	7	1014	CLA	C4B-NB-C1B	2.43	109.97	106.76
17	9	1016	CLA	C4B-NB-C1B	2.43	109.97	106.76
17	9	1021	CLA	C4B-NB-C1B	2.43	109.97	106.76
17	F	1229	CLA	C1C-NC-C4C	2.43	109.45	106.28
17	P	5138	CLA	C1C-NC-C4C	2.43	109.45	106.28
17	A	1123	CLA	C4B-NB-C1B	2.43	109.96	106.76
17	B	1232	CLA	C1C-NC-C4C	2.42	109.44	106.28
17	B	1237	CLA	C1C-NC-C4C	2.42	109.44	106.28
17	2	1014	CLA	C4B-NB-C1B	2.42	109.95	106.76
17	P	5120	CLA	C1C-NC-C4C	2.42	109.44	106.28
17	8	1031	CLA	C4B-NB-C1B	2.41	109.94	106.76
17	A	1138	CLA	C1C-NC-C4C	2.40	109.42	106.28
17	A	1012	CLA	C4B-NB-C1B	2.40	109.92	106.76
17	A	1120	CLA	C1C-NC-C4C	2.39	109.40	106.28
17	8	1014	CLA	C4B-NB-C1B	2.39	109.92	106.76
17	Q	5232	CLA	C1C-NC-C4C	2.39	109.40	106.28
17	A	1112	CLA	C1C-NC-C4C	2.39	109.40	106.28
17	P	5122	CLA	C1C-NC-C4C	2.39	109.40	106.28
17	P	5112	CLA	C1C-NC-C4C	2.38	109.39	106.28
17	P	5106	CLA	C1C-NC-C4C	2.38	109.38	106.28
17	A	1122	CLA	C1C-NC-C4C	2.38	109.38	106.28
17	A	1012	CLA	C1C-NC-C4C	2.37	109.38	106.28
17	A	1106	CLA	C1C-NC-C4C	2.37	109.37	106.28
17	Z	5302	CLA	CHD-C4C-NC	2.36	126.39	124.49
17	J	1302	CLA	CHD-C4C-NC	2.36	126.39	124.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	1302	CLA	C4D-ND-C1D	2.36	109.42	106.57
17	A	1134	CLA	C1C-NC-C4C	2.36	109.36	106.28
17	P	5012	CLA	C4B-NB-C1B	2.36	109.87	106.76
17	B	1218	CLA	C1C-NC-C4C	2.36	109.36	106.28
17	P	5134	CLA	C1C-NC-C4C	2.35	109.35	106.28
17	Q	5218	CLA	C1C-NC-C4C	2.35	109.34	106.28
17	P	5012	CLA	C1C-NC-C4C	2.34	109.34	106.28
17	P	5110	CLA	C1C-NC-C4C	2.33	109.33	106.28
17	P	5106	CLA	CHD-C4C-NC	2.33	126.36	124.49
17	Z	5302	CLA	C4D-ND-C1D	2.33	109.38	106.57
17	A	1106	CLA	CHD-C4C-NC	2.32	126.36	124.49
17	Q	5201	CLA	C1C-NC-C4C	2.32	109.31	106.28
17	P	5111	CLA	C4B-NB-C1B	2.31	109.81	106.76
17	A	1110	CLA	C1C-NC-C4C	2.31	109.30	106.28
17	A	1111	CLA	C4B-NB-C1B	2.29	109.79	106.76
17	B	1201	CLA	C1C-NC-C4C	2.29	109.27	106.28
17	B	1130	CLA	C4B-NB-C1B	2.28	109.77	106.76
17	B	1209	CLA	C1C-NC-C4C	2.28	109.25	106.28
17	Q	5130	CLA	C4B-NB-C1B	2.28	109.76	106.76
17	P	5133	CLA	C1C-NC-C4C	2.27	109.25	106.28
17	Q	5209	CLA	C1C-NC-C4C	2.27	109.24	106.28
17	B	1214	CLA	C1C-NC-C4C	2.26	109.23	106.28
17	A	1133	CLA	C1C-NC-C4C	2.26	109.23	106.28
17	Q	5214	CLA	C1C-NC-C4C	2.26	109.23	106.28
17	Q	5211	CLA	C1C-NC-C4C	2.26	109.23	106.28
17	A	1136	CLA	C1C-NC-C4C	2.25	109.22	106.28
17	B	1208	CLA	C1C-NC-C4C	2.25	109.21	106.28
17	6	5503	CLA	C1C-NC-C4C	2.25	109.21	106.28
17	Q	5208	CLA	C1C-NC-C4C	2.25	109.21	106.28
17	G	1233	CLA	C1C-NC-C4C	2.24	109.21	106.28
17	A	1104	CLA	C4B-NB-C1B	2.24	109.72	106.76
17	V	5233	CLA	C1C-NC-C4C	2.24	109.21	106.28
17	P	5102	CLA	C1C-NC-C4C	2.24	109.20	106.28
17	Q	5217	CLA	C1C-NC-C4C	2.24	109.20	106.28
17	P	5136	CLA	C1C-NC-C4C	2.23	109.20	106.28
17	L	1503	CLA	C1C-NC-C4C	2.24	109.20	106.28
17	P	5104	CLA	C4B-NB-C1B	2.23	109.71	106.76
17	A	1102	CLA	C1C-NC-C4C	2.23	109.19	106.28
17	B	1221	CLA	C1C-NC-C4C	2.23	109.19	106.28
17	Q	5221	CLA	C1C-NC-C4C	2.22	109.18	106.28
17	B	1217	CLA	C1C-NC-C4C	2.22	109.17	106.28
17	B	1211	CLA	C1C-NC-C4C	2.21	109.17	106.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1103	CLA	C4B-NB-C1B	2.21	109.67	106.76
17	A	1135	CLA	C4B-NB-C1B	2.20	109.66	106.76
17	P	5103	CLA	C4B-NB-C1B	2.19	109.65	106.76
17	P	5135	CLA	C4B-NB-C1B	2.18	109.63	106.76
17	A	1108	CLA	CHC-C1C-NC	2.17	127.54	123.45
17	B	1236	CLA	C1C-NC-C4C	2.17	109.11	106.28
17	P	5108	CLA	CHC-C1C-NC	2.17	127.53	123.45
17	Q	5236	CLA	C1C-NC-C4C	2.16	109.10	106.28
17	P	5140	CLA	C1C-NC-C4C	2.16	109.10	106.28
17	A	1140	CLA	C1C-NC-C4C	2.16	109.09	106.28
17	P	5114	CLA	C1C-NC-C4C	2.14	109.07	106.28
17	Q	5230	CLA	C1C-NC-C4C	2.14	109.07	106.28
17	P	5121	CLA	C1C-NC-C4C	2.13	109.07	106.28
17	A	1121	CLA	C1C-NC-C4C	2.13	109.07	106.28
17	A	1132	CLA	C1C-NC-C4C	2.13	109.06	106.28
17	B	1230	CLA	C1C-NC-C4C	2.13	109.06	106.28
17	K	1401	CLA	C1C-NC-C4C	2.13	109.06	106.28
17	A	1114	CLA	C1C-NC-C4C	2.13	109.06	106.28
17	Q	5022	CLA	C4B-NB-C1B	2.13	109.56	106.76
17	5	5401	CLA	C1C-NC-C4C	2.12	109.05	106.28
17	A	1138	CLA	CHD-C4C-NC	2.13	126.20	124.49
17	P	5138	CLA	CHD-C4C-NC	2.13	126.20	124.49
17	B	1216	CLA	C1C-NC-C4C	2.12	109.05	106.28
17	B	1022	CLA	C4B-NB-C1B	2.12	109.56	106.76
17	P	5111	CLA	C1C-NC-C4C	2.12	109.05	106.28
17	P	5013	CLA	C1C-NC-C4C	2.12	109.05	106.28
17	Q	5222	CLA	C1C-NC-C4C	2.11	109.04	106.28
17	Q	5216	CLA	C1C-NC-C4C	2.12	109.04	106.28
17	A	1111	CLA	C1C-NC-C4C	2.11	109.04	106.28
17	P	5132	CLA	C1C-NC-C4C	2.11	109.03	106.28
17	B	1222	CLA	C1C-NC-C4C	2.11	109.03	106.28
17	Q	5201	CLA	CHD-C4C-NC	2.10	126.18	124.49
17	A	1013	CLA	C1C-NC-C4C	2.10	109.02	106.28
17	B	1201	CLA	CHD-C4C-NC	2.09	126.17	124.49
17	A	1131	CLA	C1C-NC-C4C	2.08	109.00	106.28
17	B	1213	CLA	C1C-NC-C4C	2.08	109.00	106.28
17	B	1234	CLA	C4B-NB-C1B	2.08	109.51	106.76
17	A	1113	CLA	CHC-C1C-NC	2.08	127.36	123.45
17	P	5113	CLA	CHC-C1C-NC	2.08	127.36	123.45
17	Q	5213	CLA	C1C-NC-C4C	2.07	108.99	106.28
17	L	1501	CLA	C1C-NC-C4C	2.07	108.98	106.28
17	6	5501	CLA	C1C-NC-C4C	2.07	108.98	106.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	5234	CLA	C4B-NB-C1B	2.06	109.48	106.76
17	A	1128	CLA	C1C-NC-C4C	2.06	108.97	106.28
17	P	5131	CLA	C1C-NC-C4C	2.06	108.97	106.28
17	B	1224	CLA	C1C-NC-C4C	2.05	108.96	106.28
17	Q	5239	CLA	C1C-NC-C4C	2.05	108.96	106.28
17	P	5128	CLA	C1C-NC-C4C	2.05	108.96	106.28
17	P	5901	CLA	C4D-ND-C1D	2.05	109.04	106.57
17	B	1021	CLA	C1C-NC-C4C	2.05	108.95	106.28
17	P	5118	CLA	C4B-NB-C1B	2.04	109.46	106.76
17	A	1901	CLA	C4D-ND-C1D	2.04	109.03	106.57
17	P	5124	CLA	C1C-NC-C4C	2.04	108.94	106.28
17	A	1118	CLA	C4B-NB-C1B	2.04	109.45	106.76
17	P	5125	CLA	C1C-NC-C4C	2.03	108.93	106.28
17	A	1124	CLA	C1C-NC-C4C	2.03	108.93	106.28
17	P	5137	CLA	CHC-C1C-NC	2.03	127.26	123.45
17	Q	5238	CLA	C1C-NC-C4C	2.03	108.92	106.28
17	Q	5021	CLA	C1C-NC-C4C	2.02	108.92	106.28
17	A	1125	CLA	C1C-NC-C4C	2.02	108.92	106.28
17	Q	5224	CLA	C1C-NC-C4C	2.02	108.92	106.28
17	A	1117	CLA	C1C-NC-C4C	2.02	108.92	106.28
17	A	1137	CLA	CHC-C1C-NC	2.02	127.25	123.45
17	0	1012	CLA	C1C-NC-C4C	2.02	108.92	106.28
17	P	5109	CLA	C1C-NC-C4C	2.02	108.91	106.28
17	B	1239	CLA	C1C-NC-C4C	2.01	108.91	106.28
17	4	1012	CLA	C1C-NC-C4C	2.01	108.91	106.28
17	A	1108	CLA	CHB-C1B-NB	2.01	127.94	124.58
17	P	5108	CLA	CHB-C1B-NB	2.01	127.93	124.58
17	P	5110	CLA	C4B-NB-C1B	2.01	109.41	106.76
17	A	1109	CLA	C1C-NC-C4C	2.01	108.90	106.28
17	J	1302	CLA	CHB-C1B-NB	2.00	127.92	124.58

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.