



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 16, 2018 – 11:57 PM EDT

PDB ID : 5ZF0
Title : X-ray Structure of the Electron Transfer Complex between Ferredoxin and Photosystem I
Authors : Kubota-Kawai, H.; Mutoh, R.; Shinmura, K.; Setif, P.; Nowaczyk, M.; Roegner, M.; Ikegami, T.; Tanaka, T.; Kurisu, G.
Deposited on : 2018-03-01
Resolution : 4.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031021
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031021

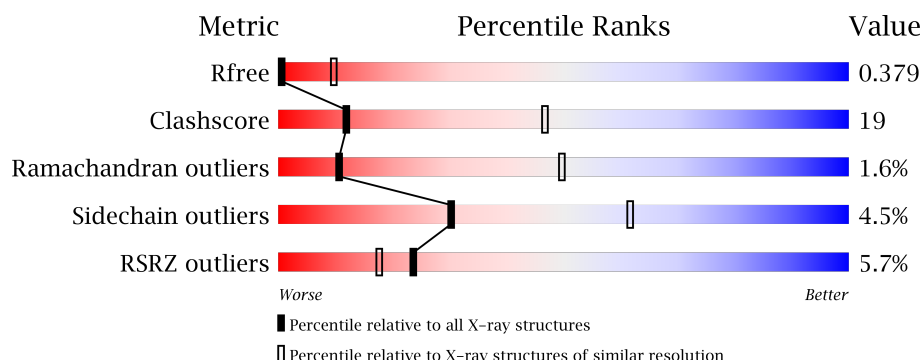
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1014 (4.70-3.70)
Clashscore	122126	1082 (4.70-3.70)
Ramachandran outliers	120053	1035 (4.70-3.70)
Sidechain outliers	120020	1021 (4.70-3.70)
RSRZ outliers	108989	1179 (4.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A1	755	<div> <div>12%</div> <div>68%</div> <div>28%</div> <div>..</div> </div>
1	A2	755	<div> <div>5%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
1	A3	755	<div> <div>4%</div> <div>69%</div> <div>27%</div> <div>..</div> </div>
1	A4	755	<div> <div>8%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
1	A5	755	<div> <div>5%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	A6	755	
2	B1	740	
2	B2	740	
2	B3	740	
2	B4	740	
2	B5	740	
2	B6	740	
3	C1	80	
3	C2	80	
3	C3	80	
3	C4	80	
3	C5	80	
3	C6	80	
4	D1	138	
4	D2	138	
4	D3	138	
4	D4	138	
4	D5	138	
4	D6	138	
5	E1	75	
5	E2	75	
5	E3	75	
5	E4	75	
5	E5	75	
5	E6	75	

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Mol	Chain	Length	Quality of chain
6	F1	164	
6	F2	164	
6	F3	164	
6	F4	164	
6	F5	164	
6	F6	164	
7	I1	38	
7	I2	38	
7	I3	38	
7	I4	38	
7	I5	38	
7	I6	38	
8	J1	41	
8	J2	41	
8	J3	41	
8	J4	41	
8	J5	41	
8	J6	41	
9	K1	83	
9	K2	83	
9	K3	83	
9	K4	83	
9	K5	83	
9	K6	83	
10	L1	154	

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Mol	Chain	Length	Quality of chain
10	L2	154	
10	L3	154	
10	L4	154	
10	L5	154	
10	L6	154	
11	M1	31	
11	M2	31	
11	M3	31	
11	M4	31	
11	M5	31	
11	M6	31	
12	X1	35	
12	X2	35	
12	X3	35	
12	X4	35	
12	X5	35	
12	X6	35	
13	P1	97	
13	P2	97	
13	P3	97	
13	P4	97	
13	P5	97	
13	P6	97	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A1	801	X	-	-	-
14	CLA	A1	802	X	-	-	X
14	CLA	A1	803	X	-	-	X
14	CLA	A1	804	X	-	-	X
14	CLA	A1	805	X	-	-	X
14	CLA	A1	806	X	-	-	-
14	CLA	A1	807	X	-	-	-
14	CLA	A1	808	X	-	-	-
14	CLA	A1	809	X	-	-	X
14	CLA	A1	810	X	-	-	X
14	CLA	A1	811	X	-	-	X
14	CLA	A1	812	X	-	-	X
14	CLA	A1	813	X	-	-	-
14	CLA	A1	814	X	-	-	X
14	CLA	A1	815	X	-	-	X
14	CLA	A1	816	X	-	-	X
14	CLA	A1	817	X	-	-	-
14	CLA	A1	818	X	-	-	-
14	CLA	A1	819	X	-	-	X
14	CLA	A1	820	X	-	-	X
14	CLA	A1	821	X	-	-	-
14	CLA	A1	822	X	-	-	-
14	CLA	A1	823	X	-	-	-
14	CLA	A1	824	X	-	-	X
14	CLA	A1	825	X	-	-	-
14	CLA	A1	826	X	-	-	X
14	CLA	A1	827	X	-	-	X
14	CLA	A1	828	X	-	-	-
14	CLA	A1	829	X	-	-	-
14	CLA	A1	830	X	-	-	-
14	CLA	A1	832	X	-	-	-
14	CLA	A1	833	X	-	-	X
14	CLA	A1	834	X	-	-	-
14	CLA	A1	835	X	-	-	-
14	CLA	A1	836	X	-	-	-
14	CLA	A1	837	X	-	-	X
14	CLA	A1	838	X	-	-	-
14	CLA	A1	839	X	-	-	-
14	CLA	A1	840	X	-	-	X
14	CLA	A2	1601	X	-	-	X
14	CLA	A2	1602	X	-	-	-
14	CLA	A2	1603	X	-	-	-
14	CLA	A2	1604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A2	1605	X	-	-	-
14	CLA	A2	1606	X	-	-	X
14	CLA	A2	1607	X	-	-	X
14	CLA	A2	1608	X	-	-	-
14	CLA	A2	1609	X	-	-	-
14	CLA	A2	1610	X	-	-	-
14	CLA	A2	1611	X	-	-	-
14	CLA	A2	1612	X	-	-	-
14	CLA	A2	1613	X	-	-	-
14	CLA	A2	1614	X	-	-	-
14	CLA	A2	1615	X	-	-	X
14	CLA	A2	1616	X	-	-	-
14	CLA	A2	1617	X	-	-	-
14	CLA	A2	1618	X	-	-	X
14	CLA	A2	1619	X	-	-	-
14	CLA	A2	1620	X	-	-	-
14	CLA	A2	1621	X	-	-	-
14	CLA	A2	1622	X	-	-	-
14	CLA	A2	1623	X	-	-	-
14	CLA	A2	1624	X	-	-	-
14	CLA	A2	1625	X	-	-	-
14	CLA	A2	1626	X	-	-	-
14	CLA	A2	1627	X	-	-	X
14	CLA	A2	1628	X	-	-	-
14	CLA	A2	1629	X	-	-	-
14	CLA	A2	1630	X	-	-	-
14	CLA	A2	1631	X	-	-	-
14	CLA	A2	1632	X	-	-	-
14	CLA	A2	1633	X	-	-	-
14	CLA	A2	1634	X	-	-	-
14	CLA	A2	1636	X	-	-	-
14	CLA	A2	1637	X	-	-	-
14	CLA	A2	1638	X	-	-	-
14	CLA	A2	1639	X	-	-	-
14	CLA	A2	1640	X	-	-	-
14	CLA	A2	1641	X	-	-	-
14	CLA	A2	1642	X	-	-	-
14	CLA	A2	1643	X	-	-	-
14	CLA	A2	1644	X	-	-	-
14	CLA	A2	1645	X	-	-	X
14	CLA	A3	802	X	-	-	-
14	CLA	A3	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A3	804	X	-	-	-
14	CLA	A3	805	X	-	-	-
14	CLA	A3	806	X	-	-	-
14	CLA	A3	807	X	-	-	-
14	CLA	A3	808	X	-	-	-
14	CLA	A3	809	X	-	-	X
14	CLA	A3	810	X	-	-	-
14	CLA	A3	811	X	-	-	-
14	CLA	A3	812	X	-	-	-
14	CLA	A3	813	X	-	-	-
14	CLA	A3	814	X	-	-	-
14	CLA	A3	815	X	-	-	-
14	CLA	A3	816	X	-	-	-
14	CLA	A3	817	X	-	-	-
14	CLA	A3	818	X	-	-	-
14	CLA	A3	819	X	-	-	-
14	CLA	A3	820	X	-	-	-
14	CLA	A3	821	X	-	-	-
14	CLA	A3	822	X	-	-	-
14	CLA	A3	823	X	-	-	-
14	CLA	A3	824	X	-	-	-
14	CLA	A3	825	X	-	-	-
14	CLA	A3	826	X	-	-	-
14	CLA	A3	827	X	-	-	-
14	CLA	A3	828	X	-	-	-
14	CLA	A3	829	X	-	-	-
14	CLA	A3	830	X	-	-	-
14	CLA	A3	831	X	-	-	-
14	CLA	A3	832	X	-	-	-
14	CLA	A3	834	X	-	-	-
14	CLA	A3	835	X	-	-	-
14	CLA	A3	836	X	-	-	-
14	CLA	A3	837	X	-	-	-
14	CLA	A3	838	X	-	-	-
14	CLA	A3	839	X	-	-	-
14	CLA	A3	840	X	-	-	-
14	CLA	A3	841	X	-	-	-
14	CLA	A3	842	X	-	-	-
14	CLA	A3	843	X	-	-	-
14	CLA	A3	844	X	-	-	-
14	CLA	A3	845	X	-	-	-
14	CLA	A4	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A4	802	X	-	-	-
14	CLA	A4	803	X	-	-	-
14	CLA	A4	804	X	-	-	X
14	CLA	A4	805	X	-	-	-
14	CLA	A4	806	X	-	-	X
14	CLA	A4	807	X	-	-	-
14	CLA	A4	808	X	-	-	-
14	CLA	A4	809	X	-	-	X
14	CLA	A4	810	X	-	-	-
14	CLA	A4	811	X	-	-	-
14	CLA	A4	812	X	-	-	-
14	CLA	A4	813	X	-	-	-
14	CLA	A4	814	X	-	-	-
14	CLA	A4	815	X	-	-	X
14	CLA	A4	816	X	-	-	X
14	CLA	A4	817	X	-	-	-
14	CLA	A4	818	X	-	-	-
14	CLA	A4	819	X	-	-	-
14	CLA	A4	820	X	-	-	-
14	CLA	A4	821	X	-	-	-
14	CLA	A4	822	X	-	-	-
14	CLA	A4	823	X	-	-	-
14	CLA	A4	824	X	-	-	X
14	CLA	A4	825	X	-	-	X
14	CLA	A4	826	X	-	-	-
14	CLA	A4	827	X	-	-	-
14	CLA	A4	828	X	-	-	-
14	CLA	A4	829	X	-	-	-
14	CLA	A4	830	X	-	-	-
14	CLA	A4	831	X	-	-	-
14	CLA	A4	833	X	-	-	-
14	CLA	A4	834	X	-	-	-
14	CLA	A4	835	X	-	-	-
14	CLA	A4	836	X	-	-	-
14	CLA	A4	838	X	-	-	-
14	CLA	A4	839	X	-	-	-
14	CLA	A4	840	X	-	-	-
14	CLA	A4	841	X	-	-	-
14	CLA	A4	842	X	-	-	X
14	CLA	A4	853	X	-	-	X
14	CLA	A5	801	X	-	-	-
14	CLA	A5	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A5	803	X	-	-	-
14	CLA	A5	804	X	-	-	-
14	CLA	A5	805	X	-	-	-
14	CLA	A5	806	X	-	-	-
14	CLA	A5	807	X	-	-	-
14	CLA	A5	808	X	-	-	-
14	CLA	A5	809	X	-	-	-
14	CLA	A5	810	X	-	-	X
14	CLA	A5	811	X	-	-	-
14	CLA	A5	812	X	-	-	-
14	CLA	A5	813	X	-	-	-
14	CLA	A5	814	X	-	-	-
14	CLA	A5	815	X	-	-	X
14	CLA	A5	816	X	-	-	X
14	CLA	A5	817	X	-	-	-
14	CLA	A5	818	X	-	-	-
14	CLA	A5	819	X	-	-	-
14	CLA	A5	820	X	-	-	-
14	CLA	A5	821	X	-	-	-
14	CLA	A5	822	X	-	-	-
14	CLA	A5	823	X	-	-	-
14	CLA	A5	824	X	-	-	-
14	CLA	A5	825	X	-	-	-
14	CLA	A5	826	X	-	-	-
14	CLA	A5	827	X	-	-	-
14	CLA	A5	828	X	-	-	-
14	CLA	A5	829	X	-	-	-
14	CLA	A5	830	X	-	-	-
14	CLA	A5	831	X	-	-	-
14	CLA	A5	832	X	-	-	-
14	CLA	A5	834	X	-	-	-
14	CLA	A5	835	X	-	-	-
14	CLA	A5	836	X	-	-	-
14	CLA	A5	837	X	-	-	-
14	CLA	A5	838	X	-	-	-
14	CLA	A5	839	X	-	-	-
14	CLA	A5	840	X	-	-	-
14	CLA	A5	841	X	-	-	-
14	CLA	A5	842	X	-	-	-
14	CLA	A5	843	X	-	-	-
14	CLA	A6	1601	X	-	-	X
14	CLA	A6	1603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A6	1604	X	-	-	-
14	CLA	A6	1605	X	-	-	-
14	CLA	A6	1606	X	-	-	-
14	CLA	A6	1607	X	-	-	-
14	CLA	A6	1608	X	-	-	-
14	CLA	A6	1609	X	-	-	-
14	CLA	A6	1610	X	-	-	X
14	CLA	A6	1611	X	-	-	-
14	CLA	A6	1612	X	-	-	-
14	CLA	A6	1613	X	-	-	-
14	CLA	A6	1614	X	-	-	-
14	CLA	A6	1615	X	-	-	-
14	CLA	A6	1616	X	-	-	-
14	CLA	A6	1617	X	-	-	-
14	CLA	A6	1618	X	-	-	-
14	CLA	A6	1619	X	-	-	-
14	CLA	A6	1620	X	-	-	-
14	CLA	A6	1621	X	-	-	-
14	CLA	A6	1622	X	-	-	-
14	CLA	A6	1623	X	-	-	-
14	CLA	A6	1624	X	-	-	-
14	CLA	A6	1625	X	-	-	-
14	CLA	A6	1626	X	-	-	-
14	CLA	A6	1627	X	-	-	-
14	CLA	A6	1628	X	-	-	-
14	CLA	A6	1629	X	-	-	-
14	CLA	A6	1630	X	-	-	-
14	CLA	A6	1631	X	-	-	-
14	CLA	A6	1633	X	-	-	-
14	CLA	A6	1634	X	-	-	-
14	CLA	A6	1635	X	-	-	-
14	CLA	A6	1636	X	-	-	-
14	CLA	A6	1637	X	-	-	-
14	CLA	A6	1638	X	-	-	-
14	CLA	A6	1639	X	-	-	-
14	CLA	A6	1640	X	-	-	-
14	CLA	A6	1641	X	-	-	-
14	CLA	A6	1651	X	-	-	-
14	CLA	B1	801	X	-	-	X
14	CLA	B1	802	X	-	-	X
14	CLA	B1	803	X	-	-	-
14	CLA	B1	804	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B1	805	X	-	-	X
14	CLA	B1	806	X	-	-	-
14	CLA	B1	807	X	-	X	-
14	CLA	B1	808	X	-	-	-
14	CLA	B1	809	X	-	-	-
14	CLA	B1	810	X	-	-	-
14	CLA	B1	812	X	-	-	-
14	CLA	B1	813	X	-	-	X
14	CLA	B1	814	X	-	-	X
14	CLA	B1	815	X	-	-	-
14	CLA	B1	816	X	-	-	-
14	CLA	B1	817	X	-	X	X
14	CLA	B1	818	X	-	X	X
14	CLA	B1	819	X	-	-	-
14	CLA	B1	820	X	-	-	X
14	CLA	B1	821	X	-	-	X
14	CLA	B1	822	X	-	-	X
14	CLA	B1	823	X	-	-	X
14	CLA	B1	824	X	-	-	X
14	CLA	B1	825	X	-	-	X
14	CLA	B1	826	X	-	-	X
14	CLA	B1	827	X	-	-	X
14	CLA	B1	828	X	-	-	-
14	CLA	B1	829	X	-	-	-
14	CLA	B1	830	X	-	-	-
14	CLA	B1	831	X	-	-	-
14	CLA	B1	832	X	-	-	-
14	CLA	B1	833	X	-	-	-
14	CLA	B1	834	X	-	-	X
14	CLA	B1	835	X	-	-	X
14	CLA	B1	836	X	-	-	-
14	CLA	B1	837	X	-	-	-
14	CLA	B1	838	X	-	-	X
14	CLA	B1	839	X	-	-	-
14	CLA	B1	840	X	-	-	X
14	CLA	B1	841	X	-	-	-
14	CLA	B1	853	X	-	-	X
14	CLA	B1	854	X	-	X	-
14	CLA	B2	801	X	-	-	-
14	CLA	B2	802	X	-	-	-
14	CLA	B2	803	X	-	-	-
14	CLA	B2	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B2	805	X	-	-	-
14	CLA	B2	806	X	-	-	-
14	CLA	B2	807	X	-	-	-
14	CLA	B2	809	X	-	-	-
14	CLA	B2	810	X	-	-	-
14	CLA	B2	811	X	-	-	-
14	CLA	B2	812	X	-	-	-
14	CLA	B2	813	X	-	-	-
14	CLA	B2	814	X	-	-	-
14	CLA	B2	815	X	-	-	X
14	CLA	B2	816	X	-	-	-
14	CLA	B2	817	X	-	-	-
14	CLA	B2	818	X	-	-	X
14	CLA	B2	819	X	-	-	-
14	CLA	B2	820	X	-	-	-
14	CLA	B2	821	X	-	-	X
14	CLA	B2	822	X	-	-	-
14	CLA	B2	823	X	-	-	-
14	CLA	B2	824	X	-	-	-
14	CLA	B2	825	X	-	-	-
14	CLA	B2	826	X	-	-	-
14	CLA	B2	827	X	-	-	-
14	CLA	B2	828	X	-	-	-
14	CLA	B2	829	X	-	-	X
14	CLA	B2	830	X	-	-	X
14	CLA	B2	831	X	-	-	-
14	CLA	B2	832	X	-	-	-
14	CLA	B2	833	X	-	-	-
14	CLA	B2	834	X	-	-	-
14	CLA	B2	835	X	-	-	-
14	CLA	B2	836	X	-	-	-
14	CLA	B2	837	X	-	-	-
14	CLA	B2	838	X	-	-	-
14	CLA	B2	839	X	-	-	-
14	CLA	B2	840	X	-	-	-
14	CLA	B3	1801	X	-	-	-
14	CLA	B3	1802	X	-	-	-
14	CLA	B3	1803	X	-	-	-
14	CLA	B3	1804	X	-	-	-
14	CLA	B3	1805	X	-	-	-
14	CLA	B3	1806	X	-	-	-
14	CLA	B3	1807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B3	1808	X	-	-	-
14	CLA	B3	1809	X	-	-	-
14	CLA	B3	1810	X	-	-	-
14	CLA	B3	1812	X	-	-	-
14	CLA	B3	1813	X	-	-	-
14	CLA	B3	1814	X	-	-	-
14	CLA	B3	1815	X	-	-	-
14	CLA	B3	1816	X	-	-	-
14	CLA	B3	1817	X	-	-	X
14	CLA	B3	1818	X	-	-	-
14	CLA	B3	1819	X	-	-	-
14	CLA	B3	1820	X	-	-	-
14	CLA	B3	1821	X	-	-	X
14	CLA	B3	1822	X	-	-	-
14	CLA	B3	1823	X	-	-	-
14	CLA	B3	1824	X	-	-	X
14	CLA	B3	1825	X	-	-	X
14	CLA	B3	1826	X	-	-	X
14	CLA	B3	1827	X	-	-	-
14	CLA	B3	1828	X	-	-	-
14	CLA	B3	1829	X	-	-	-
14	CLA	B3	1830	X	-	-	-
14	CLA	B3	1831	X	-	-	-
14	CLA	B3	1832	X	-	-	-
14	CLA	B3	1833	X	-	-	-
14	CLA	B3	1834	X	-	-	-
14	CLA	B3	1835	X	-	-	-
14	CLA	B3	1836	X	-	-	-
14	CLA	B3	1837	X	-	-	-
14	CLA	B3	1838	X	-	-	-
14	CLA	B3	1839	X	-	-	-
14	CLA	B3	1840	X	-	-	-
14	CLA	B3	1841	X	-	-	-
14	CLA	B3	1842	X	-	-	-
14	CLA	B3	1843	X	-	-	-
14	CLA	B4	801	X	-	-	-
14	CLA	B4	802	X	-	-	-
14	CLA	B4	803	X	-	-	-
14	CLA	B4	804	X	-	-	-
14	CLA	B4	805	X	-	-	-
14	CLA	B4	806	X	-	-	-
14	CLA	B4	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B4	808	X	-	-	-
14	CLA	B4	809	X	-	-	X
14	CLA	B4	810	X	-	-	-
14	CLA	B4	811	-	-	-	X
14	CLA	B4	812	X	-	-	-
14	CLA	B4	813	X	-	-	X
14	CLA	B4	814	X	-	-	-
14	CLA	B4	815	X	-	-	-
14	CLA	B4	816	X	-	-	-
14	CLA	B4	817	X	-	-	X
14	CLA	B4	818	X	-	-	-
14	CLA	B4	819	X	-	-	-
14	CLA	B4	820	X	-	-	-
14	CLA	B4	821	X	-	-	X
14	CLA	B4	822	X	-	-	-
14	CLA	B4	823	X	-	-	-
14	CLA	B4	824	X	-	-	X
14	CLA	B4	825	X	-	-	-
14	CLA	B4	826	X	-	-	-
14	CLA	B4	827	X	-	-	X
14	CLA	B4	828	X	-	-	-
14	CLA	B4	829	X	-	-	-
14	CLA	B4	830	X	-	-	-
14	CLA	B4	831	X	-	-	-
14	CLA	B4	832	X	-	-	-
14	CLA	B4	833	X	-	-	-
14	CLA	B4	834	X	-	-	-
14	CLA	B4	835	X	-	-	-
14	CLA	B4	836	X	-	-	-
14	CLA	B4	837	X	-	-	-
14	CLA	B4	838	X	-	-	-
14	CLA	B4	839	X	-	-	-
14	CLA	B4	840	X	-	-	-
14	CLA	B4	841	X	-	-	-
14	CLA	B4	842	X	-	-	-
14	CLA	B4	843	X	-	-	-
14	CLA	B4	852	X	-	-	-
14	CLA	B5	1801	X	-	-	X
14	CLA	B5	1802	X	-	-	-
14	CLA	B5	1803	X	-	X	-
14	CLA	B5	1804	X	-	-	-
14	CLA	B5	1805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B5	1806	X	-	-	-
14	CLA	B5	1807	X	-	-	-
14	CLA	B5	1808	X	-	-	-
14	CLA	B5	1809	X	-	-	-
14	CLA	B5	1810	X	-	-	-
14	CLA	B5	1812	X	-	-	-
14	CLA	B5	1813	X	-	-	X
14	CLA	B5	1814	X	-	-	X
14	CLA	B5	1815	X	-	-	X
14	CLA	B5	1816	X	-	-	-
14	CLA	B5	1817	X	-	-	X
14	CLA	B5	1818	X	-	-	X
14	CLA	B5	1819	X	-	-	X
14	CLA	B5	1820	X	-	-	-
14	CLA	B5	1821	X	-	-	X
14	CLA	B5	1822	X	-	-	X
14	CLA	B5	1823	X	-	-	X
14	CLA	B5	1824	X	-	-	-
14	CLA	B5	1825	X	-	-	-
14	CLA	B5	1826	X	-	-	X
14	CLA	B5	1827	X	-	-	X
14	CLA	B5	1828	X	-	-	-
14	CLA	B5	1829	X	-	-	-
14	CLA	B5	1830	X	-	-	-
14	CLA	B5	1831	X	-	-	-
14	CLA	B5	1832	X	-	-	-
14	CLA	B5	1833	X	-	-	-
14	CLA	B5	1834	X	-	-	-
14	CLA	B5	1835	X	-	-	-
14	CLA	B5	1836	X	-	-	X
14	CLA	B5	1837	X	-	-	-
14	CLA	B5	1838	X	-	-	-
14	CLA	B5	1839	X	-	-	X
14	CLA	B5	1840	X	-	-	-
14	CLA	B5	1841	X	-	-	-
14	CLA	B5	1842	X	-	-	-
14	CLA	B5	1843	X	-	-	-
14	CLA	B6	802	X	-	-	-
14	CLA	B6	803	X	-	-	-
14	CLA	B6	804	X	-	-	-
14	CLA	B6	805	X	-	-	-
14	CLA	B6	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B6	807	X	-	-	-
14	CLA	B6	808	X	-	-	-
14	CLA	B6	810	X	-	-	-
14	CLA	B6	811	X	-	-	-
14	CLA	B6	812	X	-	-	-
14	CLA	B6	813	X	-	-	-
14	CLA	B6	814	X	-	-	-
14	CLA	B6	815	X	-	-	-
14	CLA	B6	816	X	-	-	X
14	CLA	B6	817	X	-	-	-
14	CLA	B6	818	X	-	-	-
14	CLA	B6	819	X	-	-	X
14	CLA	B6	820	X	-	-	-
14	CLA	B6	821	X	-	-	-
14	CLA	B6	822	X	-	-	-
14	CLA	B6	823	X	-	-	X
14	CLA	B6	824	X	-	-	-
14	CLA	B6	825	X	-	-	-
14	CLA	B6	826	X	-	-	-
14	CLA	B6	827	X	-	-	-
14	CLA	B6	828	X	-	-	-
14	CLA	B6	829	X	-	-	-
14	CLA	B6	830	X	-	-	-
14	CLA	B6	831	X	-	-	X
14	CLA	B6	832	X	-	-	-
14	CLA	B6	833	X	-	-	-
14	CLA	B6	834	X	-	-	-
14	CLA	B6	835	X	-	-	-
14	CLA	B6	836	X	-	-	-
14	CLA	B6	837	X	-	-	-
14	CLA	B6	838	X	-	-	-
14	CLA	B6	839	X	-	-	-
14	CLA	B6	840	X	-	-	-
14	CLA	B6	841	X	-	-	-
14	CLA	F1	1301	X	-	-	X
14	CLA	F2	202	X	-	-	-
14	CLA	F2	204	X	-	-	X
14	CLA	F3	202	X	-	-	X
14	CLA	F4	202	X	-	-	X
14	CLA	F5	1301	X	-	-	X
14	CLA	F6	202	X	-	-	X
14	CLA	I1	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	I6	101	X	-	-	-
14	CLA	J1	101	X	-	-	X
14	CLA	J1	102	X	-	-	X
14	CLA	J2	101	X	-	-	-
14	CLA	J3	101	X	-	-	-
14	CLA	J3	102	X	-	-	X
14	CLA	J4	101	X	-	-	X
14	CLA	J4	102	X	-	-	-
14	CLA	J5	101	X	-	-	X
14	CLA	J5	102	X	-	-	-
14	CLA	J6	1101	X	-	-	-
14	CLA	J6	1102	X	-	-	-
14	CLA	J6	1103	X	-	-	-
14	CLA	K1	1401	X	-	-	X
14	CLA	K2	1401	X	-	-	-
14	CLA	K3	1401	X	-	-	-
14	CLA	K4	1401	X	-	-	-
14	CLA	K5	101	X	-	-	-
14	CLA	K5	102	X	-	-	-
14	CLA	K6	1401	X	-	-	-
14	CLA	L1	201	X	-	-	-
14	CLA	L1	202	X	-	-	-
14	CLA	L1	205	X	-	-	-
14	CLA	L1	206	X	-	-	-
14	CLA	L1	207	X	-	-	-
14	CLA	L2	202	X	-	-	-
14	CLA	L2	205	X	-	-	-
14	CLA	L2	206	X	-	-	-
14	CLA	L2	207	X	-	-	-
14	CLA	L3	202	X	-	-	X
14	CLA	L3	203	X	-	-	-
14	CLA	L3	204	X	-	-	-
14	CLA	L3	205	X	-	-	X
14	CLA	L4	201	X	-	-	-
14	CLA	L4	203	X	-	-	-
14	CLA	L4	204	X	-	-	-
14	CLA	L4	205	X	-	-	-
14	CLA	L5	202	X	-	-	X
14	CLA	L5	203	X	-	-	-
14	CLA	L5	204	X	-	-	-
14	CLA	L5	205	X	-	-	-
14	CLA	L5	206	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	L6	202	X	-	-	-
14	CLA	L6	203	X	-	-	-
14	CLA	L6	206	X	-	-	-
14	CLA	L6	207	X	-	-	-
14	CLA	L6	208	X	-	-	-
14	CLA	M1	1201	X	-	-	-
14	CLA	M2	1201	X	-	-	-
14	CLA	M3	1601	X	-	-	X
14	CLA	M6	1201	X	-	-	-
14	CLA	X1	1701	X	-	-	-
14	CLA	X2	1701	X	-	-	-
14	CLA	X3	102	X	-	-	X
14	CLA	X4	102	X	-	-	-
14	CLA	X5	101	X	-	-	X
14	CLA	X6	1701	X	-	-	-
15	PQN	A1	841	-	-	-	X
15	PQN	A2	1646	-	-	-	X
15	PQN	A4	843	-	-	-	X
15	PQN	A5	844	-	-	-	X
15	PQN	B3	1844	-	-	-	X
15	PQN	B4	844	-	-	-	X
15	PQN	B5	1844	-	-	-	X
16	BCR	A1	842	-	-	-	X
16	BCR	A1	843	-	-	-	X
16	BCR	A1	844	-	-	-	X
16	BCR	A1	845	-	-	-	X
16	BCR	A1	846	-	-	-	X
16	BCR	A1	847	-	-	-	X
16	BCR	A2	1647	-	-	-	X
16	BCR	A2	1648	-	-	-	X
16	BCR	A2	1649	-	-	-	X
16	BCR	A2	1650	-	-	-	X
16	BCR	A2	1651	-	-	-	X
16	BCR	A2	1652	-	-	-	X
16	BCR	A3	847	-	-	-	X
16	BCR	A3	849	-	-	-	X
16	BCR	A3	850	-	-	-	X
16	BCR	A4	844	-	-	-	X
16	BCR	A4	845	-	-	-	X
16	BCR	A4	846	-	-	-	X
16	BCR	A4	847	-	-	-	X
16	BCR	A4	848	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	BCR	A4	849	-	-	-	X
16	BCR	A5	845	-	-	-	X
16	BCR	A5	846	-	-	-	X
16	BCR	A5	847	-	-	-	X
16	BCR	A5	848	-	-	-	X
16	BCR	A5	849	-	-	-	X
16	BCR	A5	850	-	-	-	X
16	BCR	A5	853	-	-	-	X
16	BCR	A6	1643	-	-	-	X
16	BCR	A6	1644	-	-	-	X
16	BCR	A6	1645	-	-	-	X
16	BCR	A6	1646	-	-	-	X
16	BCR	A6	1648	-	-	-	X
16	BCR	B1	843	-	-	-	X
16	BCR	B1	844	-	-	-	X
16	BCR	B1	845	-	-	-	X
16	BCR	B1	846	-	-	-	X
16	BCR	B1	847	-	-	-	X
16	BCR	B1	848	-	-	-	X
16	BCR	B1	849	-	-	-	X
16	BCR	B1	852	-	-	-	X
16	BCR	B2	842	-	-	-	X
16	BCR	B2	843	-	-	-	X
16	BCR	B2	844	-	-	-	X
16	BCR	B2	845	-	-	-	X
16	BCR	B2	846	-	-	-	X
16	BCR	B3	1845	-	-	-	X
16	BCR	B3	1846	-	-	-	X
16	BCR	B3	1847	-	-	-	X
16	BCR	B3	1848	-	-	-	X
16	BCR	B3	1849	-	-	-	X
16	BCR	B3	1851	-	-	-	X
16	BCR	B4	845	-	-	-	X
16	BCR	B4	846	-	-	-	X
16	BCR	B4	847	-	-	-	X
16	BCR	B4	848	-	-	-	X
16	BCR	B4	849	-	-	-	X
16	BCR	B4	850	-	-	-	X
16	BCR	B5	1845	-	-	-	X
16	BCR	B5	1846	-	-	-	X
16	BCR	B5	1847	-	-	-	X
16	BCR	B5	1848	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	BCR	B5	1849	-	-	-	X
16	BCR	B5	1850	-	-	-	X
16	BCR	B6	843	-	-	-	X
16	BCR	B6	844	-	-	-	X
16	BCR	B6	845	-	-	-	X
16	BCR	B6	846	-	-	-	X
16	BCR	B6	847	-	-	-	X
16	BCR	B6	850	-	-	-	X
16	BCR	F1	1302	-	-	-	X
16	BCR	F2	203	-	-	-	X
16	BCR	F3	201	-	-	-	X
16	BCR	F3	203	-	-	-	X
16	BCR	F4	201	-	-	-	X
16	BCR	F4	203	-	-	-	X
16	BCR	F4	204	-	-	-	X
16	BCR	F6	201	-	-	-	X
16	BCR	F6	203	-	-	-	X
16	BCR	I2	101	-	-	-	X
16	BCR	I4	101	-	-	-	X
16	BCR	I4	102	-	-	-	X
16	BCR	I5	101	-	-	-	X
16	BCR	J1	103	-	-	-	X
16	BCR	J1	104	-	-	-	X
16	BCR	J2	103	-	-	-	X
16	BCR	J3	104	-	-	-	X
16	BCR	J4	103	-	-	-	X
16	BCR	J4	104	-	-	-	X
16	BCR	J5	103	-	-	-	X
16	BCR	J5	104	-	-	-	X
16	BCR	J5	105	-	-	-	X
16	BCR	J6	1104	-	-	-	X
16	BCR	J6	1105	-	-	-	X
16	BCR	L1	209	-	-	-	X
16	BCR	L2	203	-	-	-	X
16	BCR	L3	201	-	-	-	X
16	BCR	L4	208	-	-	-	X
16	BCR	L5	201	-	-	-	X
16	BCR	L6	201	-	-	-	X
16	BCR	M1	1202	-	-	-	X
16	BCR	M3	1602	-	-	-	X
16	BCR	M4	101	-	-	-	X
16	BCR	M5	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	BCR	M6	1202	-	-	-	X
17	LHG	A1	848	-	-	-	X
17	LHG	A1	849	X	-	-	-
17	LHG	A2	1653	-	-	-	X
17	LHG	A2	1654	X	-	-	-
17	LHG	A3	854	X	-	-	-
17	LHG	A4	850	-	-	-	X
17	LHG	A4	851	X	-	-	-
17	LHG	A5	851	-	-	-	X
17	LHG	A5	852	X	-	-	-
17	LHG	A6	1650	X	-	-	-
17	LHG	B1	851	-	-	-	X
17	LHG	B6	849	-	-	-	X
17	LHG	X4	101	-	-	-	X
18	SF4	A1	850	-	-	X	-
18	SF4	A2	1655	-	-	X	-
18	SF4	A3	855	-	-	X	-
18	SF4	A4	852	-	-	X	-
18	SF4	A5	854	-	-	X	-
18	SF4	B6	801	-	-	X	-
18	SF4	C1	101	-	-	X	-
18	SF4	C1	102	-	-	X	-
18	SF4	C2	101	-	-	X	-
18	SF4	C2	102	-	-	X	-
18	SF4	C3	101	-	-	X	-
18	SF4	C3	102	-	-	X	-
18	SF4	C4	101	-	-	X	-
18	SF4	C4	102	-	-	X	-
18	SF4	C5	101	-	-	X	-
18	SF4	C5	102	-	-	X	-
18	SF4	C6	101	-	-	X	-
18	SF4	C6	102	-	-	X	-
19	LMG	B1	850	-	-	-	X
19	LMG	B2	848	-	-	-	X
19	LMG	B3	1850	-	-	-	X
19	LMG	B4	851	-	-	-	X
19	LMG	B5	1851	-	-	-	X
19	LMG	B6	848	-	-	-	X
20	CA	L2	204	-	-	-	X
20	CA	L6	205	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 148494 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A1	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			
1	A2	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			
1	A3	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			
1	A4	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			
1	A6	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			
1	A5	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B1	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			
2	B2	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			
2	B3	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			
2	B4	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			
2	B6	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			
2	B5	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C1	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			
3	C2	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			
3	C3	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			
3	C4	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			
3	C6	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			
3	C5	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D1	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			
4	D2	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			
4	D3	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			
4	D4	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			
4	D6	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			
4	D5	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E1	69	Total	C	N	O	0	0	0
			539	342	93	104			
5	E2	69	Total	C	N	O	0	0	0
			539	342	93	104			
5	E3	69	Total	C	N	O	0	0	0
			539	342	93	104			
5	E4	69	Total	C	N	O	0	0	0
			539	342	93	104			
5	E6	69	Total	C	N	O	0	0	0
			539	342	93	104			
5	E5	69	Total	C	N	O	0	0	0
			539	342	93	104			

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F1	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			
6	F2	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			
6	F3	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			
6	F4	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			
6	F6	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			
6	F5	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I1	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			
7	I2	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			
7	I3	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			
7	I4	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			
7	I6	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			
7	I5	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J1	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			
8	J2	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			
8	J3	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			
8	J4	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			
8	J6	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J5	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K1	46	Total	C	N	O		0	0	0
			222	130	46	46				
9	K2	46	Total	C	N	O		0	0	0
			222	130	46	46				
9	K3	46	Total	C	N	O		0	0	0
			222	130	46	46				
9	K4	46	Total	C	N	O		0	0	0
			222	130	46	46				
9	K6	46	Total	C	N	O		0	0	0
			222	130	46	46				
9	K5	46	Total	C	N	O		0	0	0
			222	130	46	46				

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L1	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			
10	L2	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			
10	L3	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			
10	L4	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			
10	L6	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			
10	L5	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L1	143	LEU	SER	conflict	UNP Q8DGB4
L2	143	LEU	SER	conflict	UNP Q8DGB4
L3	143	LEU	SER	conflict	UNP Q8DGB4
L4	143	LEU	SER	conflict	UNP Q8DGB4

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Chain	Residue	Modelled	Actual	Comment	Reference
L6	143	LEU	SER	conflict	UNP Q8DGB4
L5	143	LEU	SER	conflict	UNP Q8DGB4

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M1	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			
11	M2	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			
11	M3	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			
11	M4	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			
11	M6	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			
11	M5	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			

- Molecule 12 is a protein called Psax.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X1	29	Total	C	N	O	0	0	0
			233	164	34	35			
12	X2	29	Total	C	N	O	0	0	0
			233	164	34	35			
12	X3	29	Total	C	N	O	0	0	0
			233	164	34	35			
12	X4	29	Total	C	N	O	0	0	0
			233	164	34	35			
12	X6	29	Total	C	N	O	0	0	0
			233	164	34	35			
12	X5	29	Total	C	N	O	0	0	0
			233	164	34	35			

- Molecule 13 is a protein called Ferredoxin-1.

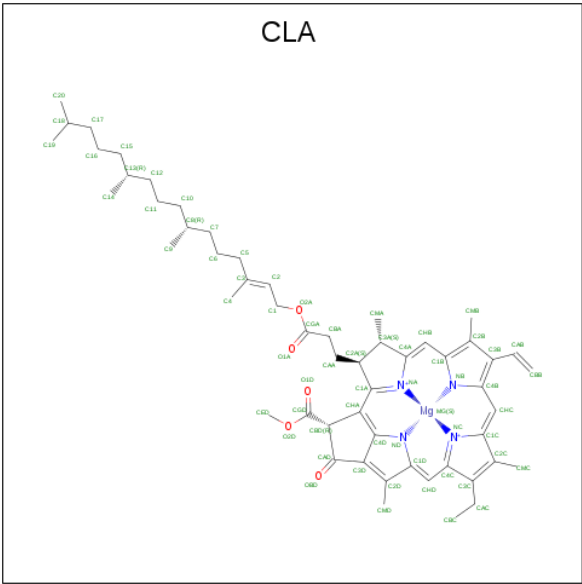
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P1	97	Total	C	N	O	S	0	0	0
			748	463	116	164	5			
13	P2	97	Total	C	N	O	S	0	0	0
			748	463	116	164	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P3	97	Total	C	N	O	S	0	0	0
			748	463	116	164	5			
13	P4	97	Total	C	N	O	S	0	0	0
			748	463	116	164	5			
13	P6	97	Total	C	N	O	S	0	0	0
			748	463	116	164	5			
13	P5	97	Total	C	N	O	S	0	0	0
			748	463	116	164	5			

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A1	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
14	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	F1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	I1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	J1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	J1	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
14	K1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	L1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	L1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	M1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	X1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
14	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	B2	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
14	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	F2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	F2	1	Total 37	C 31	Mg 1	N 4	O 1	0	0
14	J2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	K2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	L2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	L2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	L2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	L2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	M2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
14	X2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	A3	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	A3	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	A3	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	A3	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
14	A3	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	A3	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A3	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A3	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	A3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	F3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	J3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	J3	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
14	K3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	L3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	L3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	M3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	X3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A4	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A4	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	A4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
14	F4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	J4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	J4	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
14	K4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	L4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	X4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A6	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A6	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	A6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B6	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	F6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	I6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	J6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	J6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	J6	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
14	K6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	L6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	M6	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	X6	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A5	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A5	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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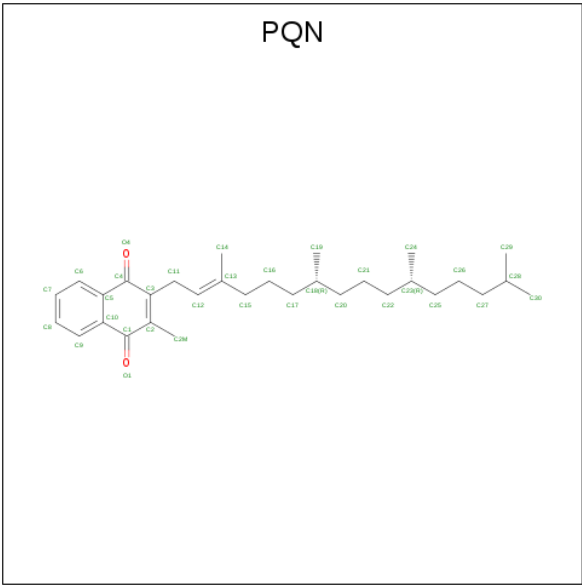
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	F5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	J5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	J5	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
14	K5	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	K5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	L5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	L5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	L5	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	X5	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



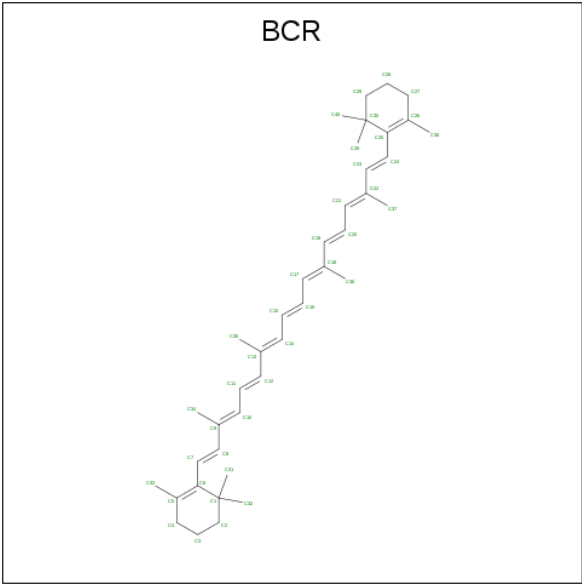
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A1	1	Total	C	O	0	0
			33	31	2		
15	B1	1	Total	C	O	0	0
			33	31	2		
15	A2	1	Total	C	O	0	0
			33	31	2		
15	B2	1	Total	C	O	0	0
			33	31	2		
15	A3	1	Total	C	O	0	0
			33	31	2		
15	B3	1	Total	C	O	0	0
			33	31	2		
15	A4	1	Total	C	O	0	0
			33	31	2		
15	B4	1	Total	C	O	0	0
			33	31	2		
15	A6	1	Total	C	O	0	0
			33	31	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B6	1	Total	C	O	0	0
			33	31	2		
15	A5	1	Total	C	O	0	0
			33	31	2		
15	B5	1	Total	C	O	0	0
			33	31	2		

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A1	1	Total	C	0	0
			40	40		
16	A1	1	Total	C	0	0
			40	40		
16	A1	1	Total	C	0	0
			40	40		
16	A1	1	Total	C	0	0
			40	40		
16	A1	1	Total	C	0	0
			40	40		
16	B1	1	Total	C	0	0
			40	40		
16	B1	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B1	1	Total C 40 40	0	0
16	B1	1	Total C 25 25	0	0
16	B1	1	Total C 40 40	0	0
16	B1	1	Total C 40 40	0	0
16	B1	1	Total C 40 40	0	0
16	B1	1	Total C 40 40	0	0
16	F1	1	Total C 40 40	0	0
16	I1	1	Total C 40 40	0	0
16	I1	1	Total C 40 40	0	0
16	J1	1	Total C 40 40	0	0
16	J1	1	Total C 40 40	0	0
16	L1	1	Total C 40 40	0	0
16	L1	1	Total C 40 40	0	0
16	M1	1	Total C 40 40	0	0
16	A2	1	Total C 40 40	0	0
16	A2	1	Total C 40 40	0	0
16	A2	1	Total C 40 40	0	0
16	A2	1	Total C 40 40	0	0
16	A2	1	Total C 40 40	0	0
16	A2	1	Total C 40 40	0	0
16	B2	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B2	1	Total C 40 40	0	0
16	B2	1	Total C 40 40	0	0
16	B2	1	Total C 25 25	0	0
16	B2	1	Total C 40 40	0	0
16	B2	1	Total C 40 40	0	0
16	B2	1	Total C 40 40	0	0
16	F2	1	Total C 40 40	0	0
16	F2	1	Total C 40 40	0	0
16	I2	1	Total C 40 40	0	0
16	J2	1	Total C 40 40	0	0
16	J2	1	Total C 40 40	0	0
16	L2	1	Total C 40 40	0	0
16	L2	1	Total C 40 40	0	0
16	L2	1	Total C 40 40	0	0
16	M2	1	Total C 40 40	0	0
16	A3	1	Total C 40 40	0	0
16	A3	1	Total C 40 40	0	0
16	A3	1	Total C 40 40	0	0
16	A3	1	Total C 40 40	0	0
16	A3	1	Total C 40 40	0	0
16	A3	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A3	1	Total C 40 40	0	0
16	B3	1	Total C 40 40	0	0
16	B3	1	Total C 40 40	0	0
16	B3	1	Total C 40 40	0	0
16	B3	1	Total C 25 25	0	0
16	B3	1	Total C 40 40	0	0
16	B3	1	Total C 40 40	0	0
16	F3	1	Total C 40 40	0	0
16	F3	1	Total C 40 40	0	0
16	I3	1	Total C 40 40	0	0
16	I3	1	Total C 40 40	0	0
16	J3	1	Total C 40 40	0	0
16	J3	1	Total C 40 40	0	0
16	L3	1	Total C 40 40	0	0
16	L3	1	Total C 40 40	0	0
16	M3	1	Total C 40 40	0	0
16	A4	1	Total C 40 40	0	0
16	A4	1	Total C 40 40	0	0
16	A4	1	Total C 40 40	0	0
16	A4	1	Total C 40 40	0	0
16	A4	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A4	1	Total C 40 40	0	0
16	B4	1	Total C 40 40	0	0
16	B4	1	Total C 40 40	0	0
16	B4	1	Total C 40 40	0	0
16	B4	1	Total C 25 25	0	0
16	B4	1	Total C 40 40	0	0
16	B4	1	Total C 40 40	0	0
16	F4	1	Total C 40 40	0	0
16	F4	1	Total C 40 40	0	0
16	F4	1	Total C 40 40	0	0
16	I4	1	Total C 40 40	0	0
16	I4	1	Total C 40 40	0	0
16	J4	1	Total C 40 40	0	0
16	J4	1	Total C 40 40	0	0
16	L4	1	Total C 40 40	0	0
16	L4	1	Total C 40 40	0	0
16	M4	1	Total C 40 40	0	0
16	A6	1	Total C 40 40	0	0
16	A6	1	Total C 40 40	0	0
16	A6	1	Total C 40 40	0	0
16	A6	1	Total C 40 40	0	0

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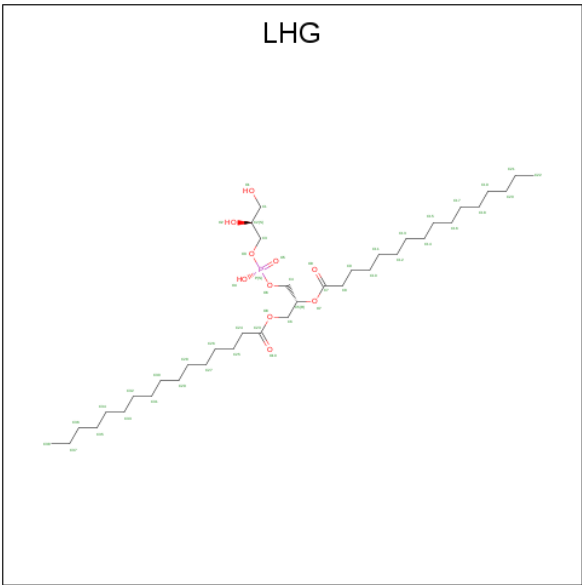
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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16	A6	1	Total C 40 40	0	0
16	A6	1	Total C 40 40	0	0
16	B6	1	Total C 40 40	0	0
16	B6	1	Total C 40 40	0	0
16	B6	1	Total C 40 40	0	0
16	B6	1	Total C 25 25	0	0
16	B6	1	Total C 40 40	0	0
16	B6	1	Total C 40 40	0	0
16	F6	1	Total C 40 40	0	0
16	F6	1	Total C 40 40	0	0
16	I6	1	Total C 40 40	0	0
16	J6	1	Total C 40 40	0	0
16	J6	1	Total C 40 40	0	0
16	L6	1	Total C 40 40	0	0
16	L6	1	Total C 40 40	0	0
16	L6	1	Total C 40 40	0	0
16	M6	1	Total C 40 40	0	0
16	A5	1	Total C 40 40	0	0
16	A5	1	Total C 40 40	0	0
16	A5	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A5	1	Total C 40 40	0	0
16	A5	1	Total C 40 40	0	0
16	A5	1	Total C 40 40	0	0
16	A5	1	Total C 40 40	0	0
16	B5	1	Total C 40 40	0	0
16	B5	1	Total C 40 40	0	0
16	B5	1	Total C 40 40	0	0
16	B5	1	Total C 25 25	0	0
16	B5	1	Total C 40 40	0	0
16	B5	1	Total C 40 40	0	0
16	F5	1	Total C 40 40	0	0
16	I5	1	Total C 40 40	0	0
16	I5	1	Total C 40 40	0	0
16	J5	1	Total C 40 40	0	0
16	J5	1	Total C 40 40	0	0
16	J5	1	Total C 40 40	0	0
16	L5	1	Total C 40 40	0	0
16	L5	1	Total C 40 40	0	0
16	M5	1	Total C 40 40	0	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



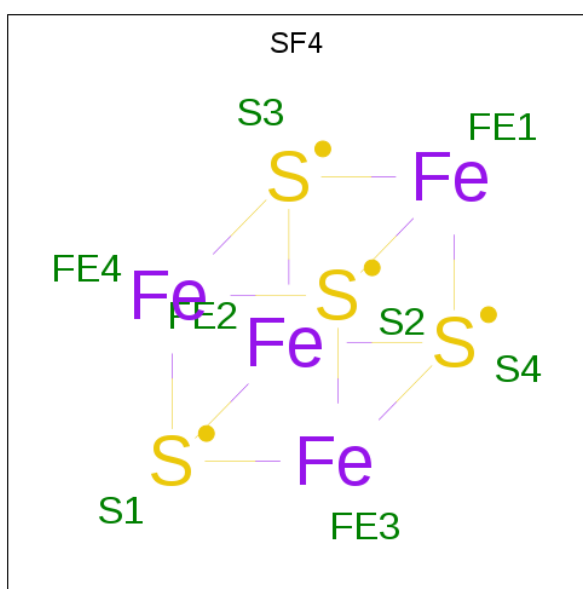
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A1	1	Total	C	O	P	0	0
			49	38	10	1		
17	A1	1	Total	C	O	P	0	0
			27	16	10	1		
17	B1	1	Total	C	O	P	0	0
			23	12	10	1		
17	A2	1	Total	C	O	P	0	0
			49	38	10	1		
17	A2	1	Total	C	O	P	0	0
			27	16	10	1		
17	B2	1	Total	C	O	P	0	0
			23	12	10	1		
17	A3	1	Total	C	O	P	0	0
			49	38	10	1		
17	A3	1	Total	C	O	P	0	0
			27	16	10	1		
17	X3	1	Total	C	O	P	0	0
			23	12	10	1		
17	A4	1	Total	C	O	P	0	0
			49	38	10	1		
17	A4	1	Total	C	O	P	0	0
			27	16	10	1		
17	X4	1	Total	C	O	P	0	0
			23	12	10	1		
17	A6	1	Total	C	O	P	0	0
			49	38	10	1		
17	A6	1	Total	C	O	P	0	0
			27	16	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B6	1	Total	C	O	P	0	0
			23	12	10	1		
17	A5	1	Total	C	O	P	0	0
			49	38	10	1		
17	A5	1	Total	C	O	P	0	0
			27	16	10	1		
17	X5	1	Total	C	O	P	0	0
			23	12	10	1		

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



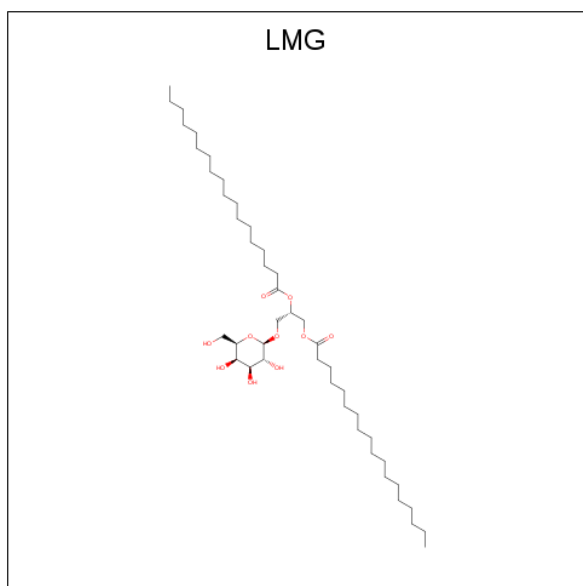
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A1	1	Total	Fe	S	0	0
			8	4	4		
18	C1	1	Total	Fe	S	0	0
			8	4	4		
18	C1	1	Total	Fe	S	0	0
			8	4	4		
18	A2	1	Total	Fe	S	0	0
			8	4	4		
18	C2	1	Total	Fe	S	0	0
			8	4	4		
18	C2	1	Total	Fe	S	0	0
			8	4	4		
18	A3	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C3	1	Total	Fe	S	0	0
			8	4	4		
18	C3	1	Total	Fe	S	0	0
			8	4	4		
18	A4	1	Total	Fe	S	0	0
			8	4	4		
18	C4	1	Total	Fe	S	0	0
			8	4	4		
18	C4	1	Total	Fe	S	0	0
			8	4	4		
18	B6	1	Total	Fe	S	0	0
			8	4	4		
18	C6	1	Total	Fe	S	0	0
			8	4	4		
18	C6	1	Total	Fe	S	0	0
			8	4	4		
18	A5	1	Total	Fe	S	0	0
			8	4	4		
18	C5	1	Total	Fe	S	0	0
			8	4	4		
18	C5	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

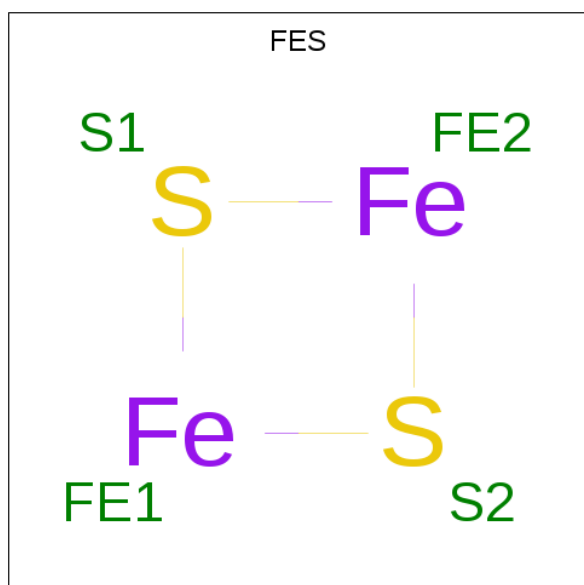


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	B1	1	Total C O 55 45 10	0	0
19	B2	1	Total C O 55 45 10	0	0
19	B3	1	Total C O 55 45 10	0	0
19	B4	1	Total C O 55 45 10	0	0
19	B6	1	Total C O 55 45 10	0	0
19	B5	1	Total C O 55 45 10	0	0

- Molecule 20 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	L6	1	Total Ca 1 1	0	0
20	L4	2	Total Ca 2 2	0	0
20	L1	2	Total Ca 2 2	0	0
20	L2	1	Total Ca 1 1	0	0

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

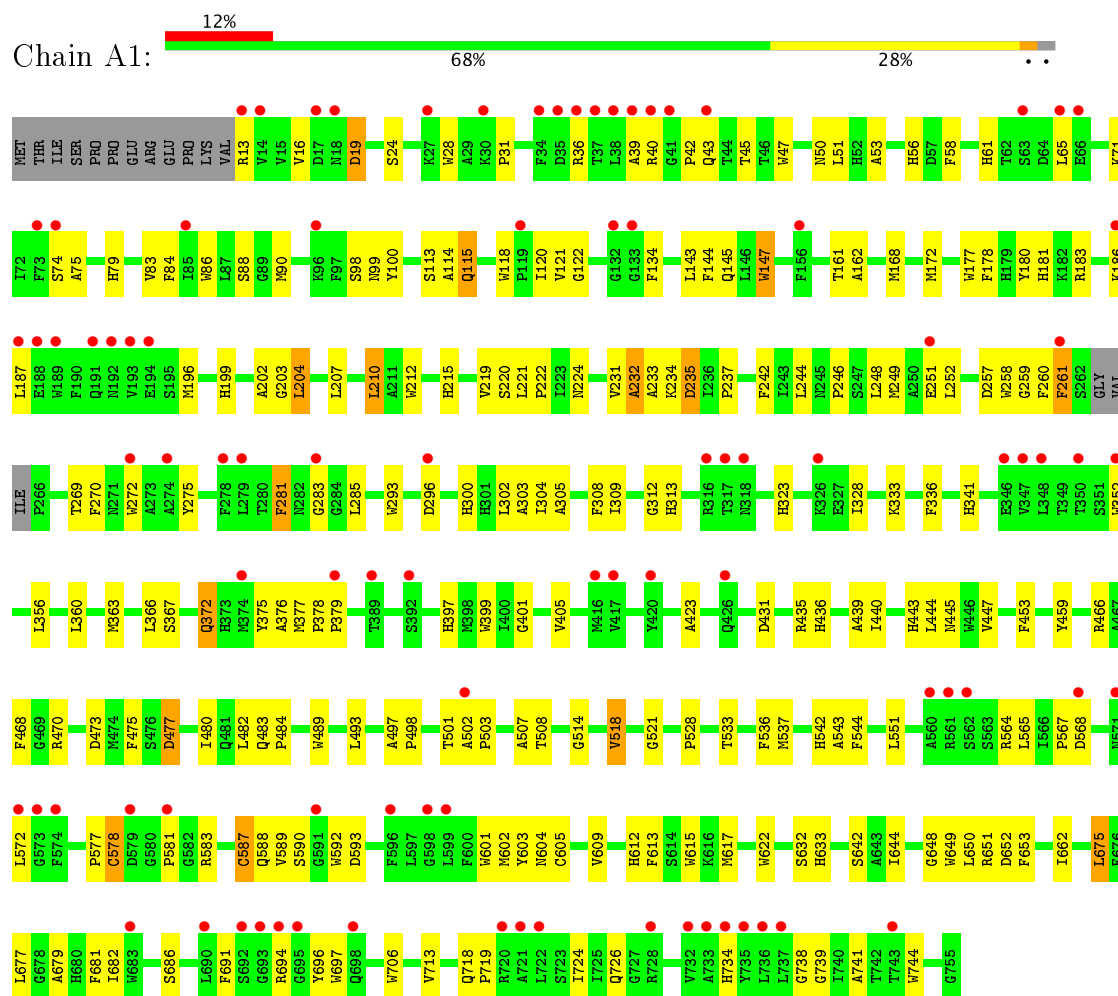


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	P1	1	Total 4	Fe 2	S 2	0	0
21	P2	1	Total 4	Fe 2	S 2	0	0
21	P3	1	Total 4	Fe 2	S 2	0	0
21	P4	1	Total 4	Fe 2	S 2	0	0
21	P6	1	Total 4	Fe 2	S 2	0	0
21	P5	1	Total 4	Fe 2	S 2	0	0

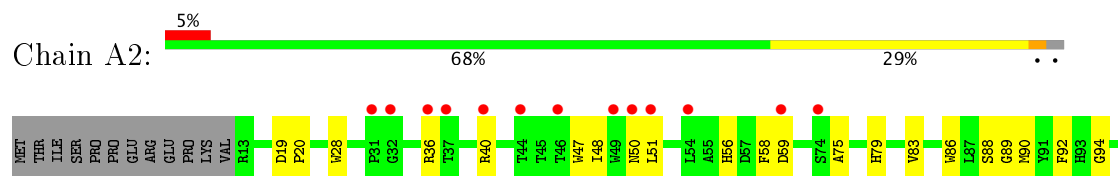
3 Residue-property plots

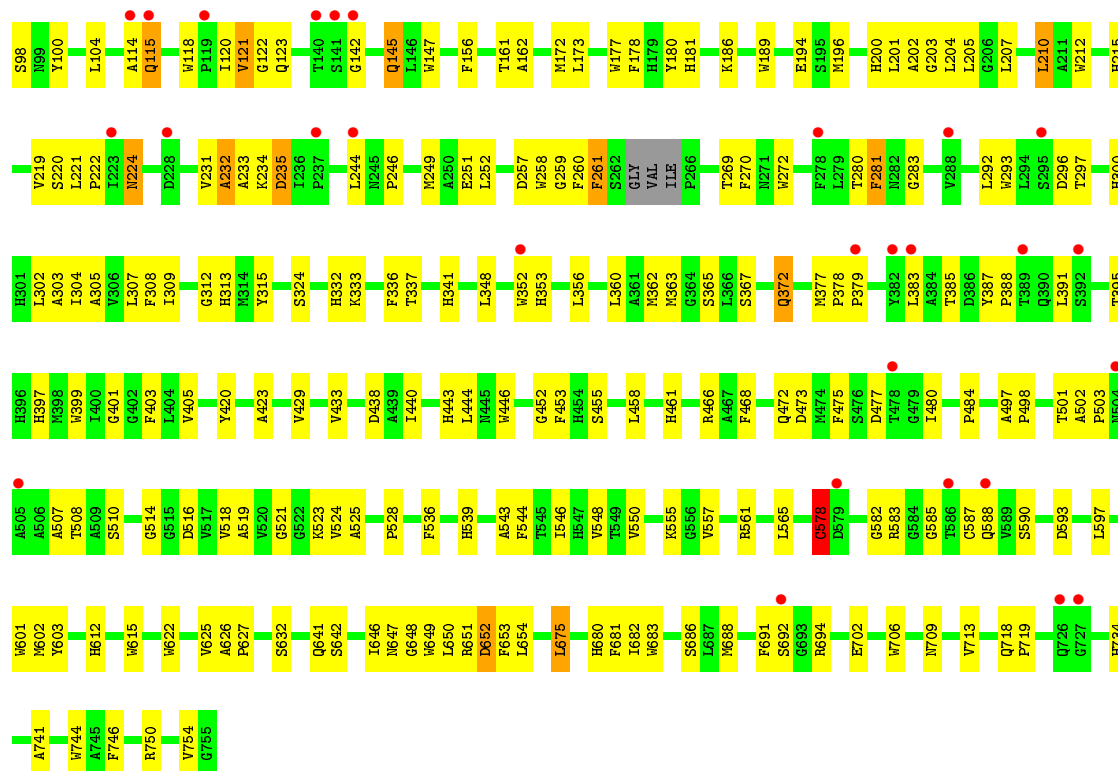
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

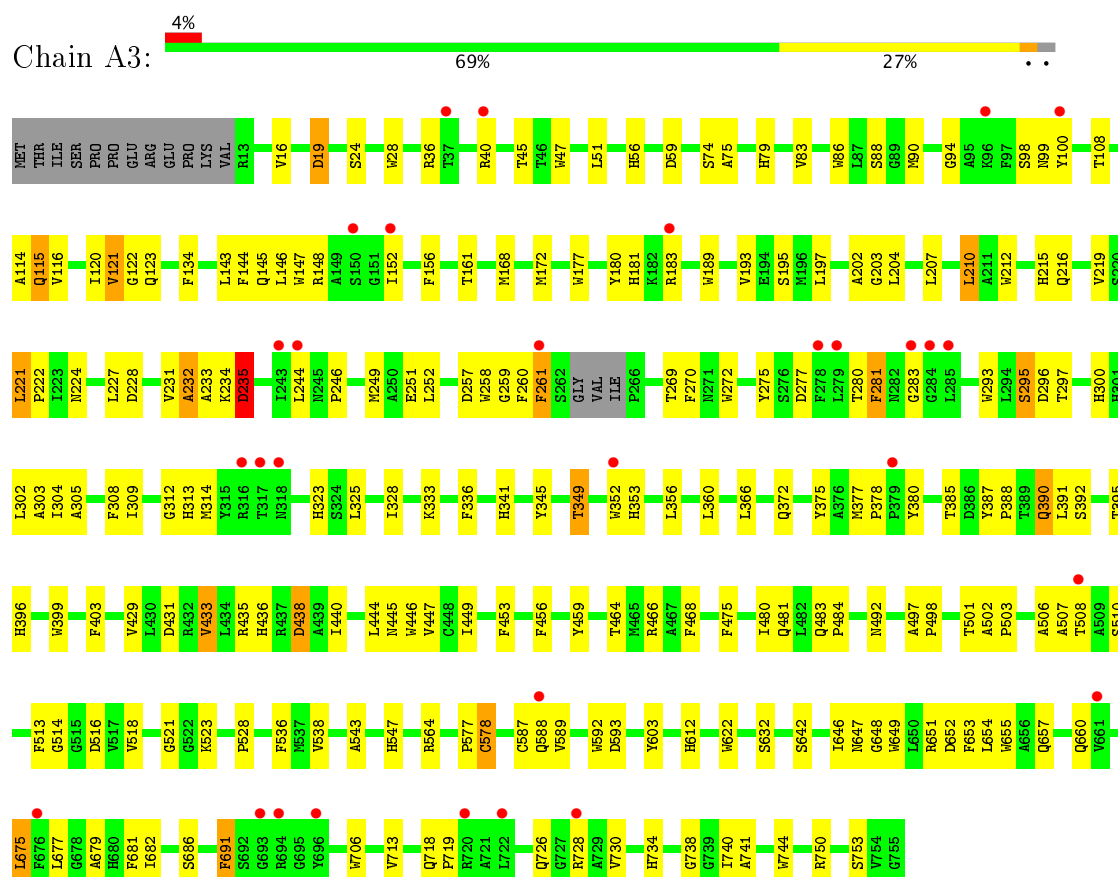


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

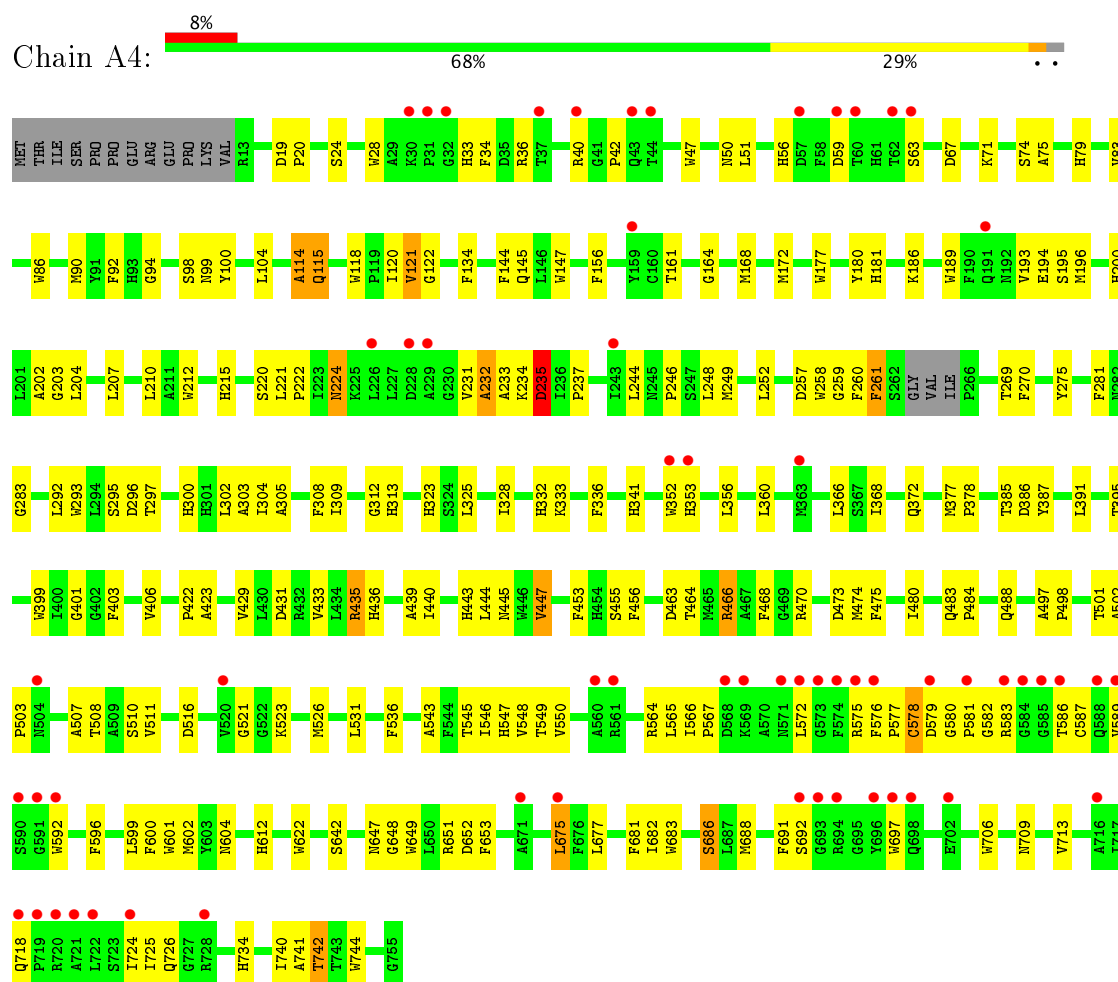




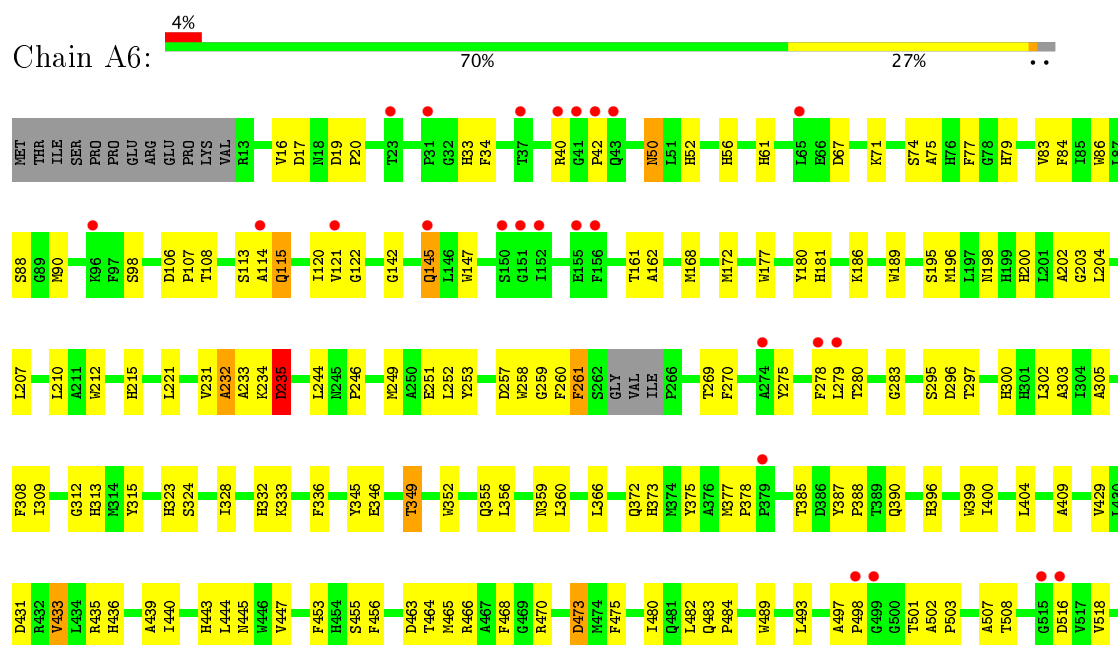
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

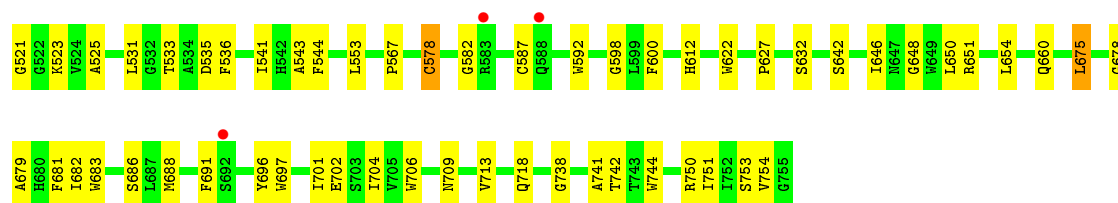


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

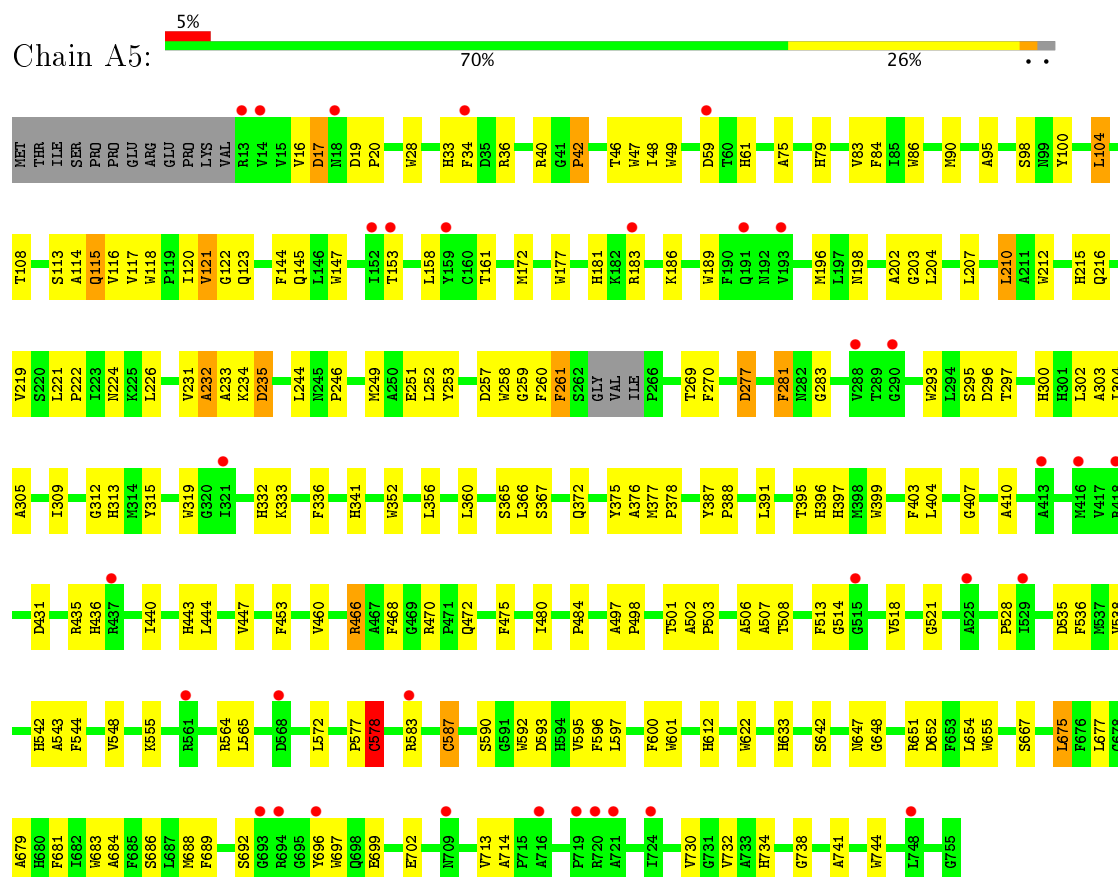


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

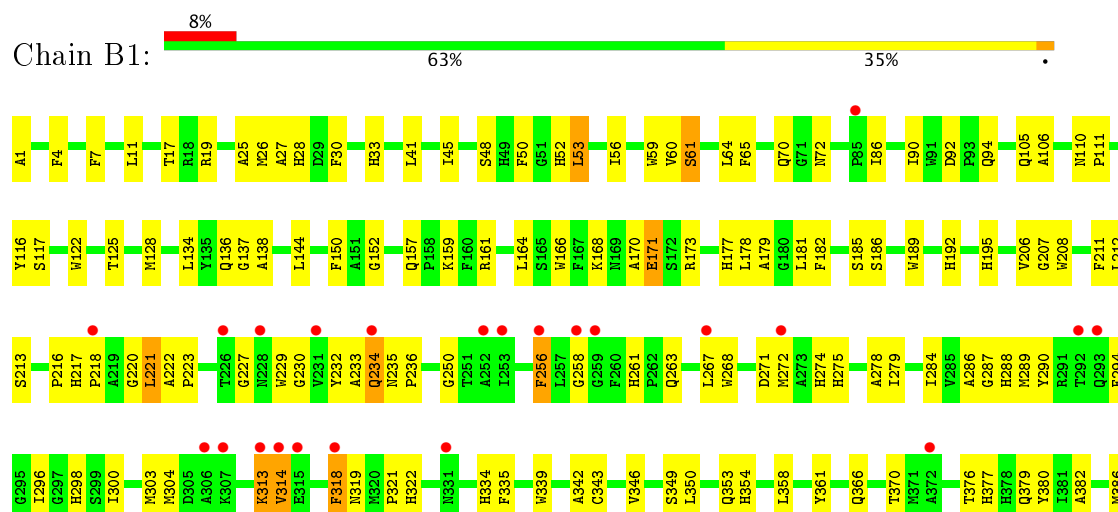


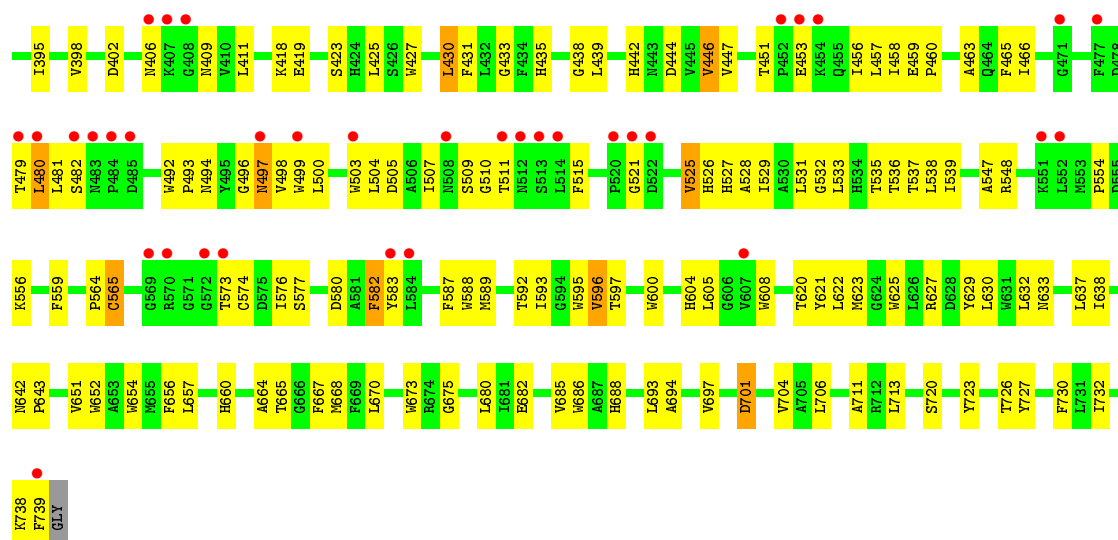


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

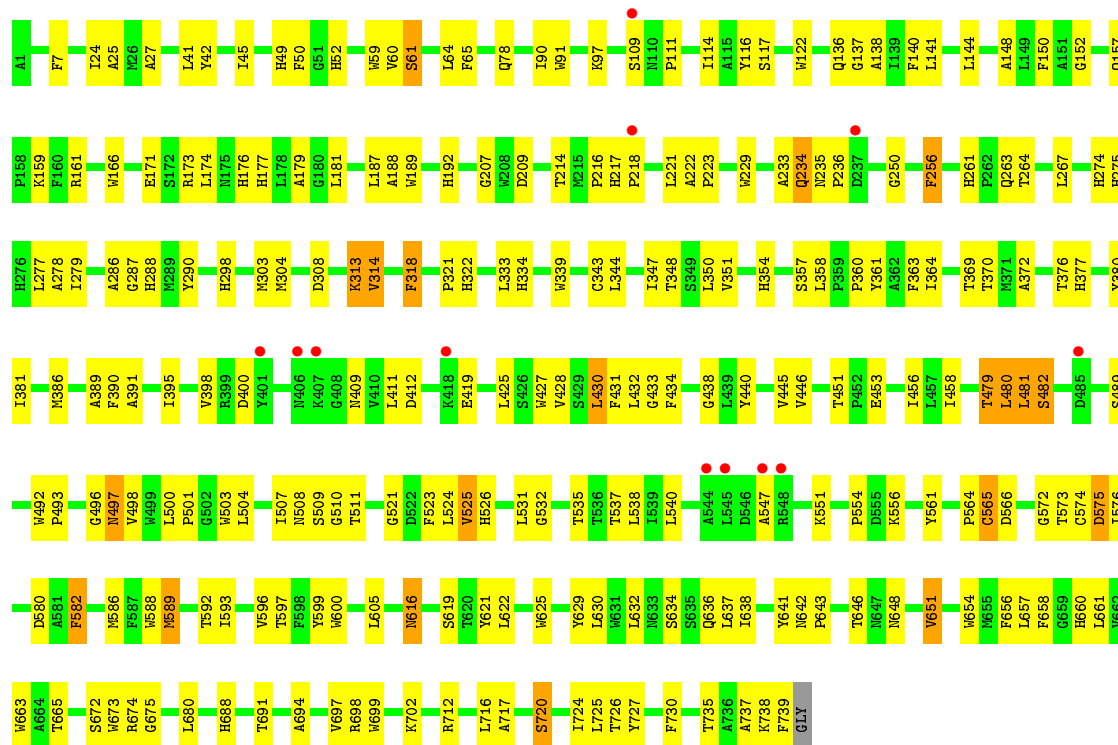


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



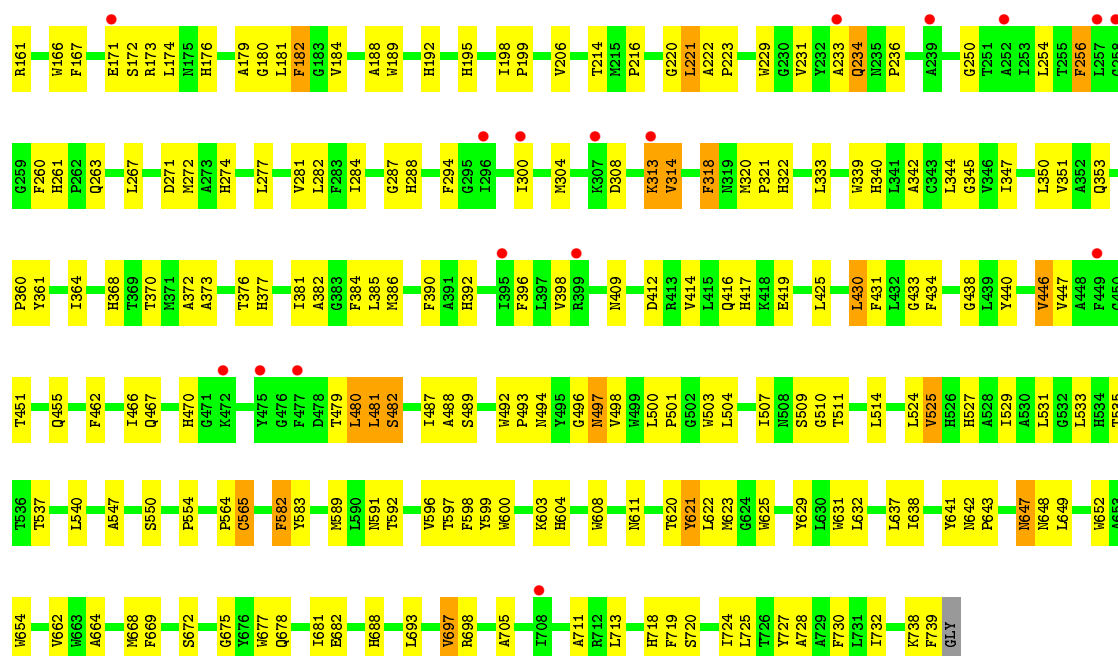


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

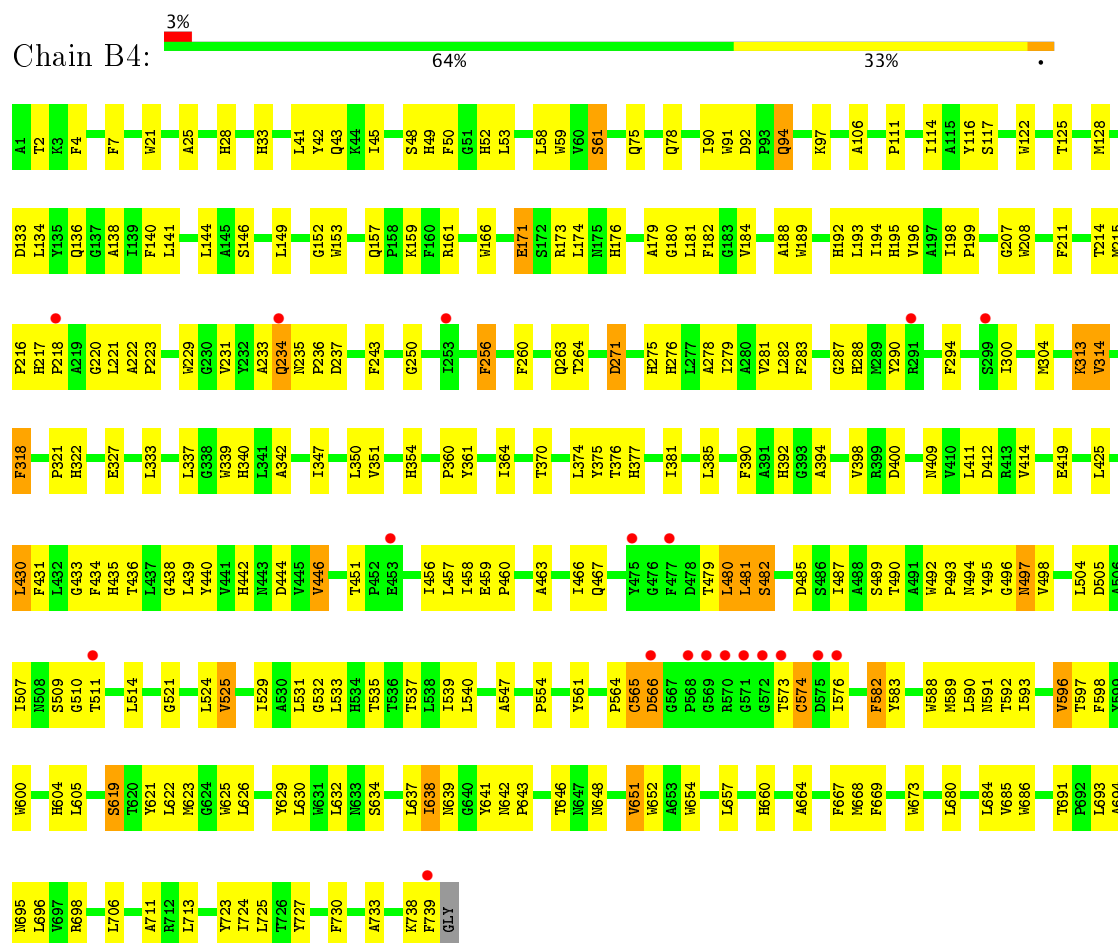


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

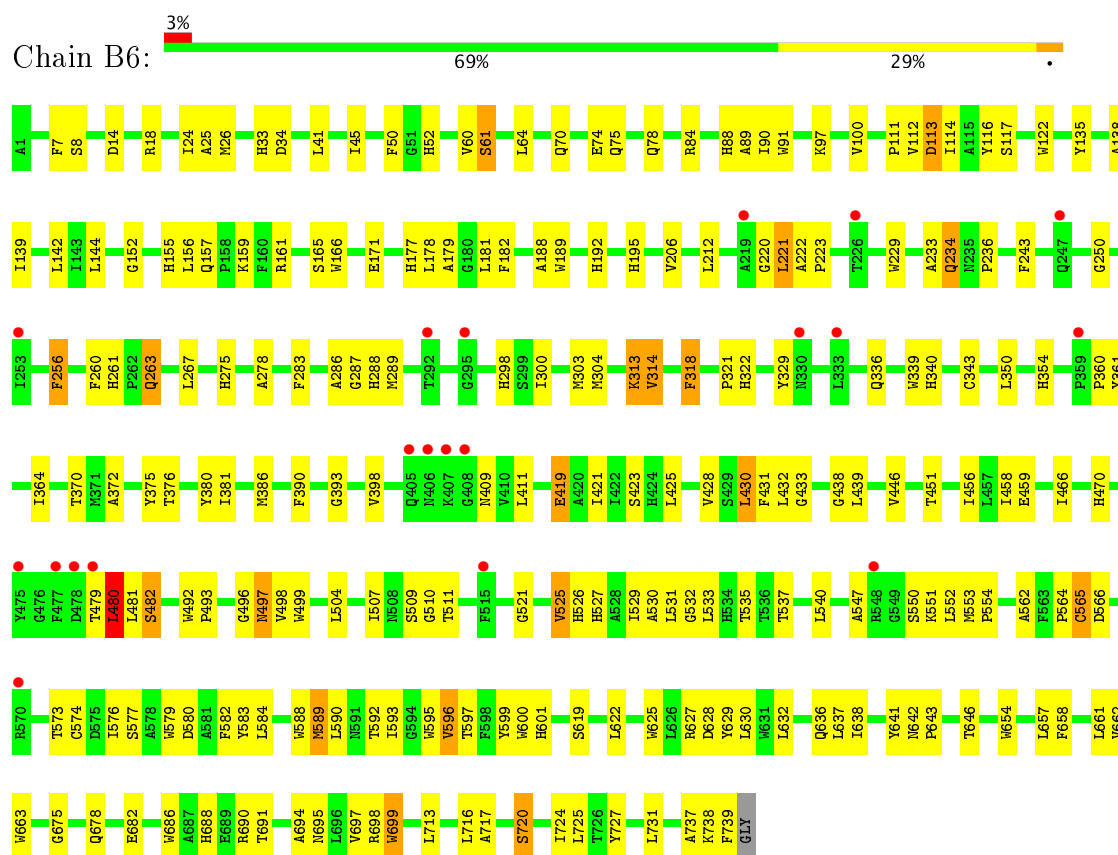




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



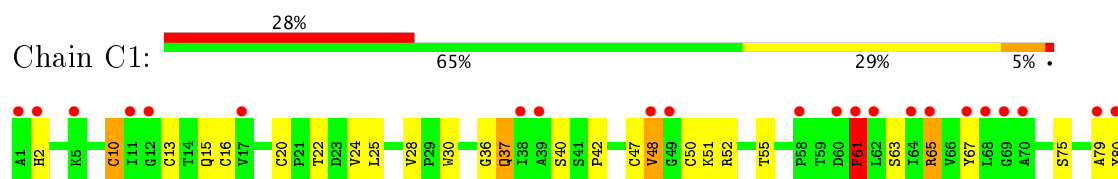
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



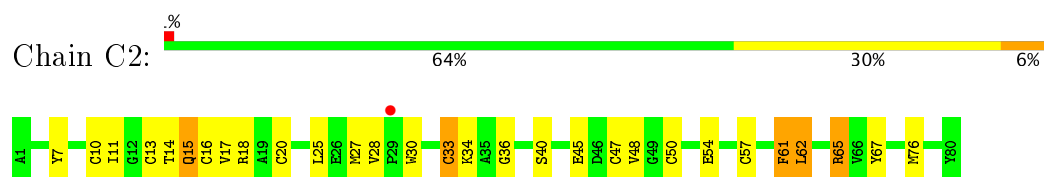
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



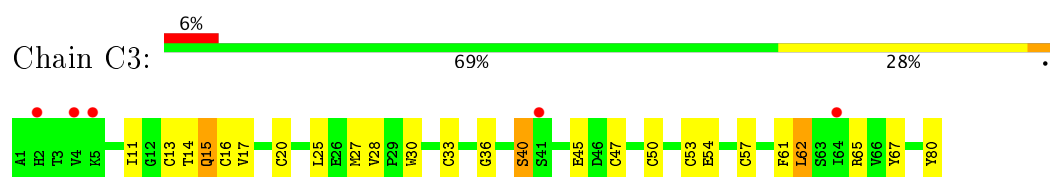
- Molecule 3: Photosystem I iron-sulfur center



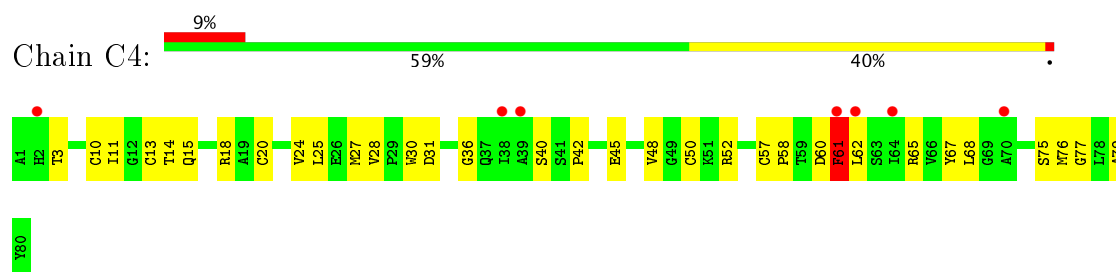
- Molecule 3: Photosystem I iron-sulfur center



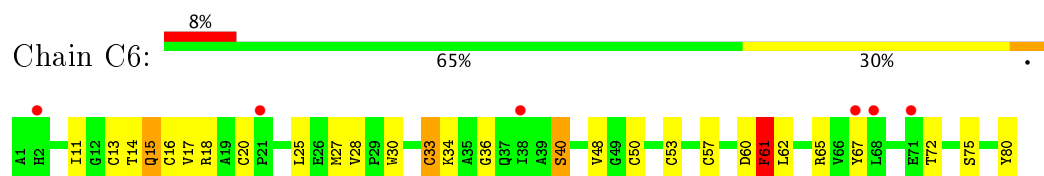
- Molecule 3: Photosystem I iron-sulfur center



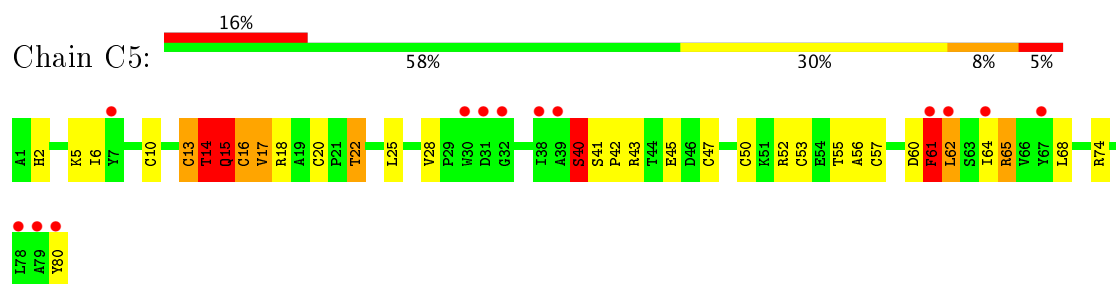
- Molecule 3: Photosystem I iron-sulfur center



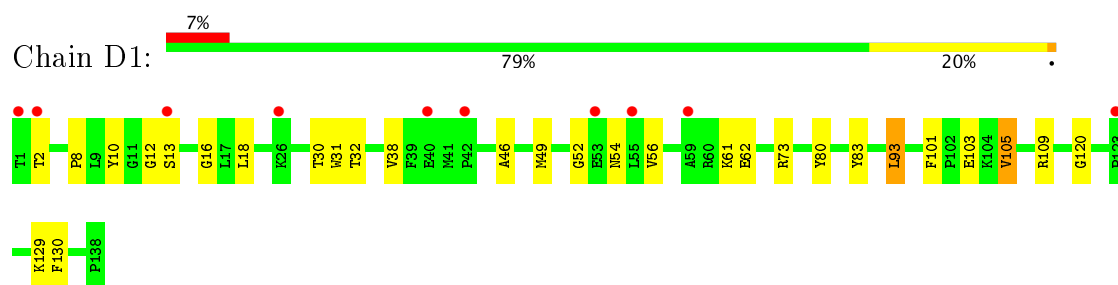
- Molecule 3: Photosystem I iron-sulfur center



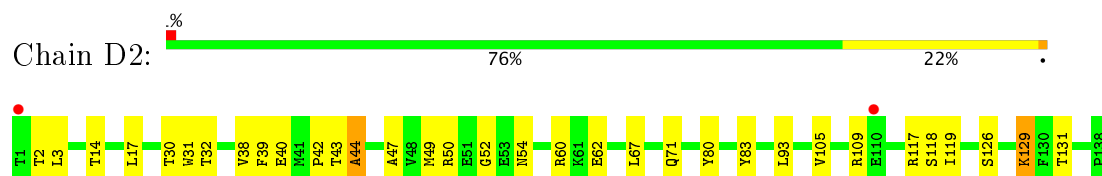
- Molecule 3: Photosystem I iron-sulfur center



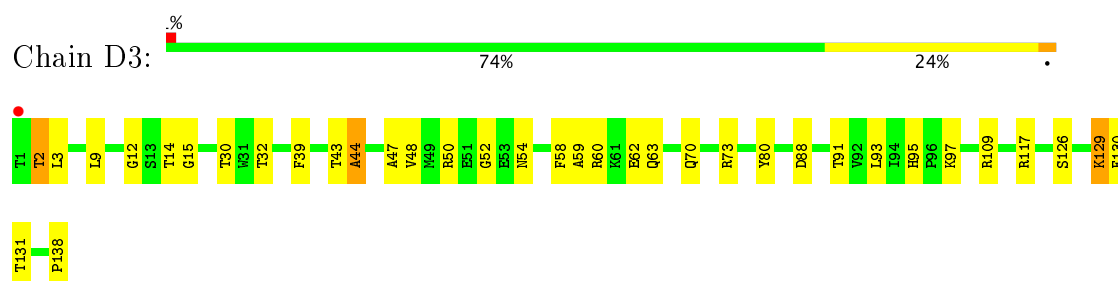
- Molecule 4: Photosystem I reaction center subunit II



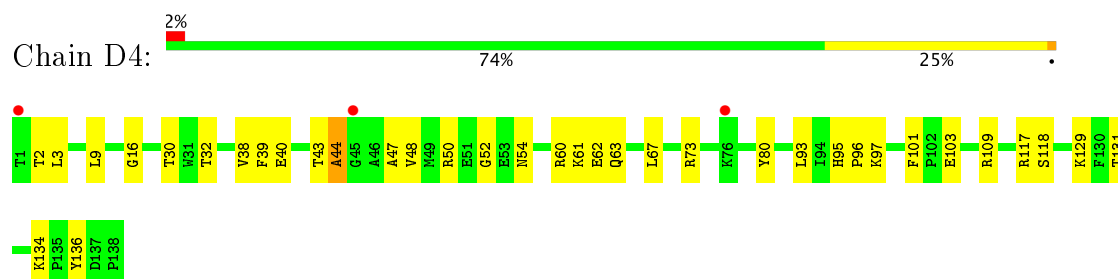
- Molecule 4: Photosystem I reaction center subunit II



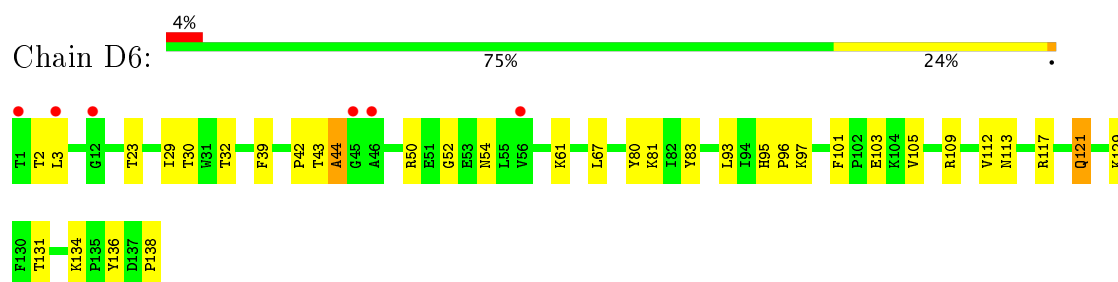
- Molecule 4: Photosystem I reaction center subunit II



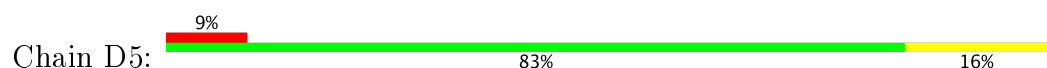
- Molecule 4: Photosystem I reaction center subunit II

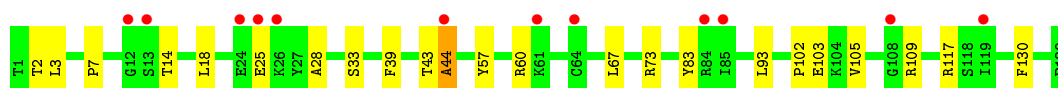


- Molecule 4: Photosystem I reaction center subunit II

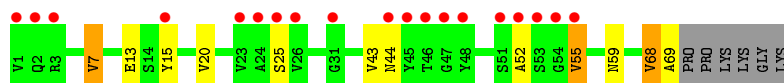
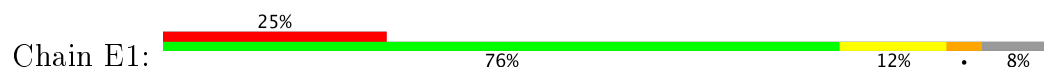


- Molecule 4: Photosystem I reaction center subunit II

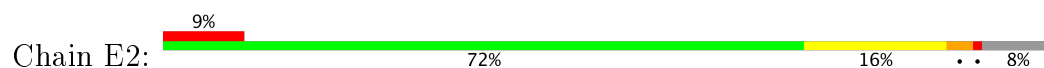




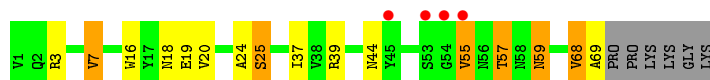
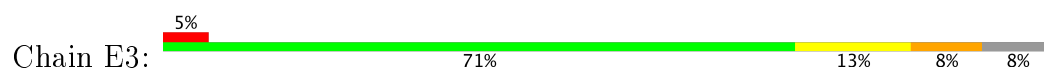
• Molecule 5: Photosystem I reaction center subunit IV



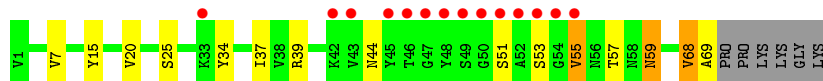
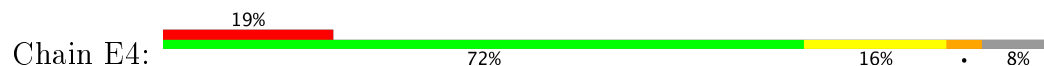
• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 5: Photosystem I reaction center subunit IV



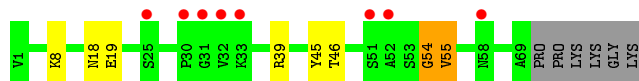
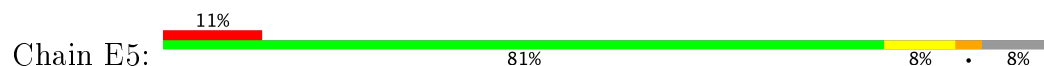
• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 5: Photosystem I reaction center subunit IV

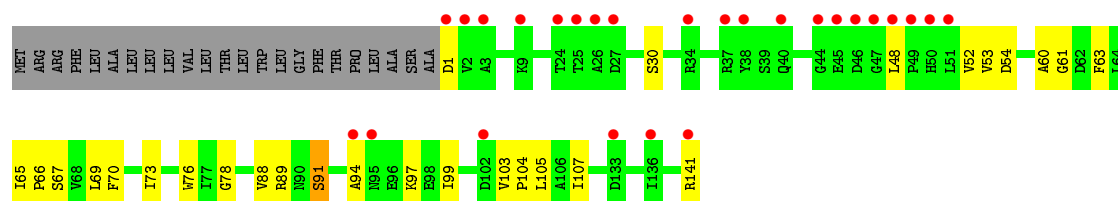


• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III

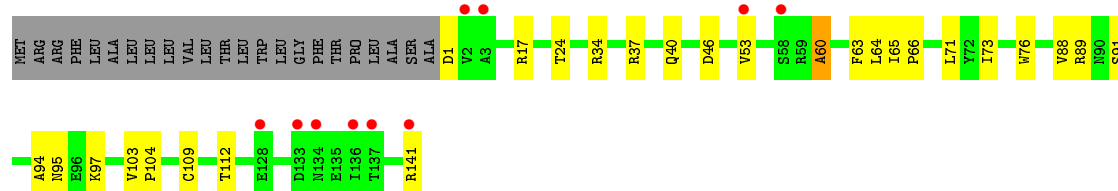




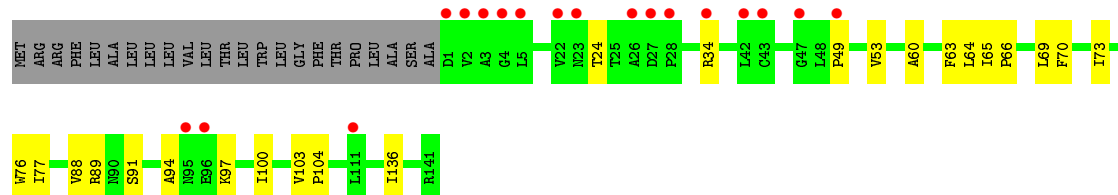
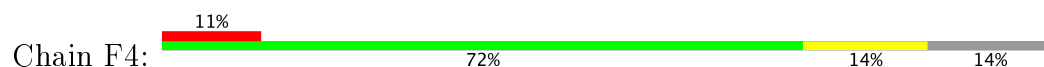
• Molecule 6: Photosystem I reaction center subunit III



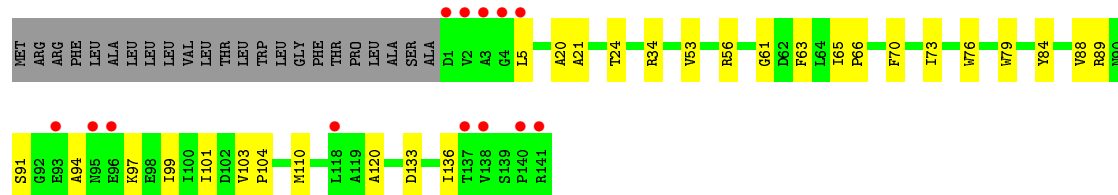
• Molecule 6: Photosystem I reaction center subunit III



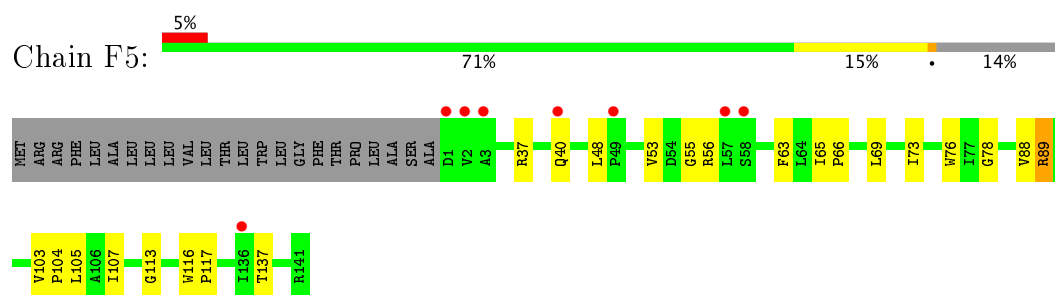
• Molecule 6: Photosystem I reaction center subunit III



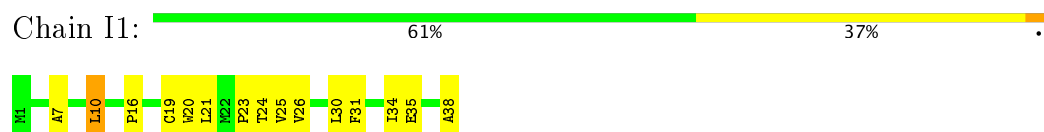
• Molecule 6: Photosystem I reaction center subunit III



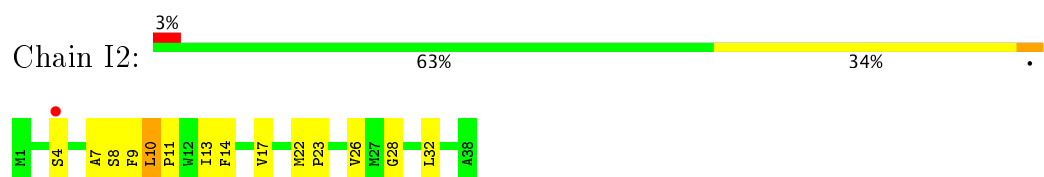
• Molecule 6: Photosystem I reaction center subunit III



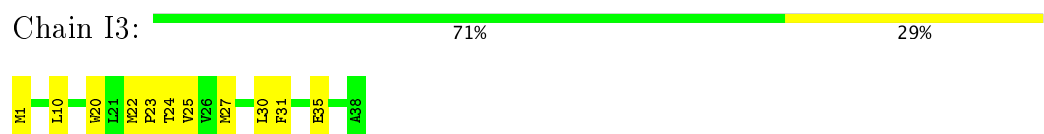
- Molecule 7: Photosystem I reaction center subunit VIII



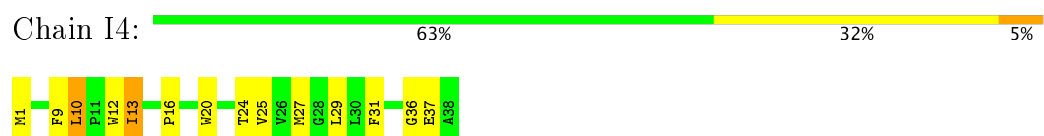
- Molecule 7: Photosystem I reaction center subunit VIII



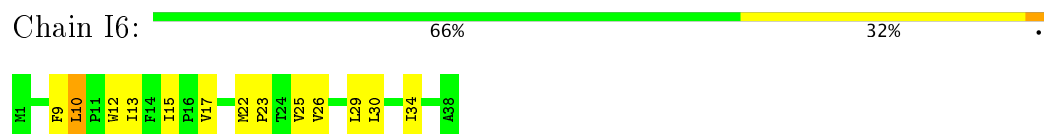
- Molecule 7: Photosystem I reaction center subunit VIII



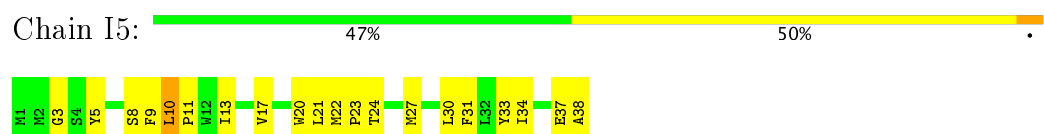
- Molecule 7: Photosystem I reaction center subunit VIII



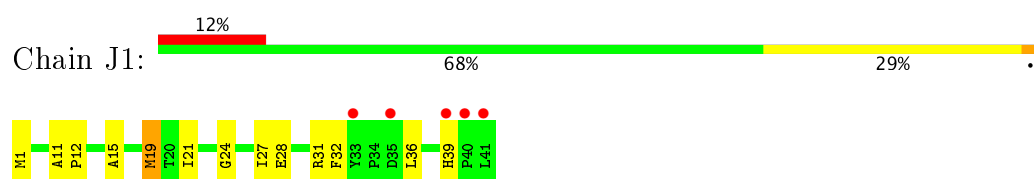
- Molecule 7: Photosystem I reaction center subunit VIII



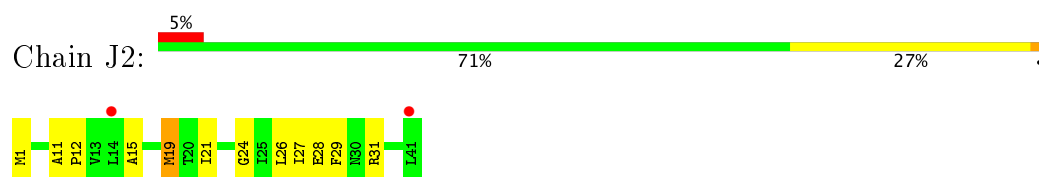
- Molecule 7: Photosystem I reaction center subunit VIII



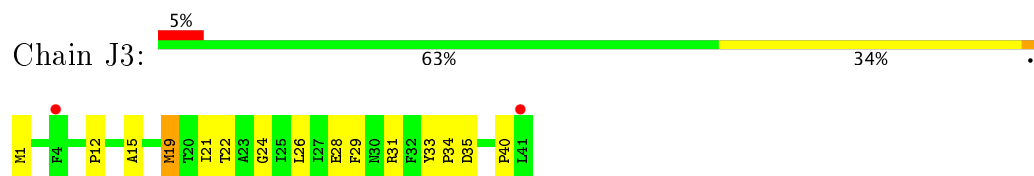
- Molecule 8: Photosystem I reaction center subunit IX



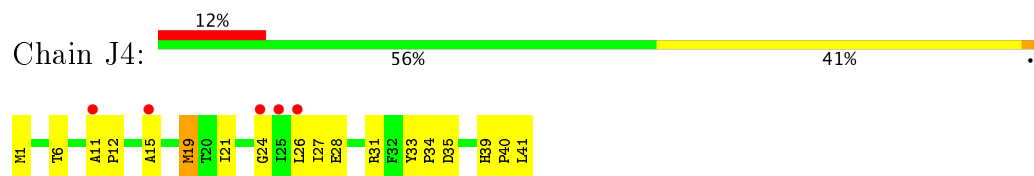
- Molecule 8: Photosystem I reaction center subunit IX



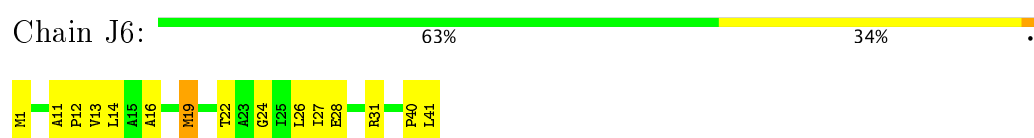
- Molecule 8: Photosystem I reaction center subunit IX



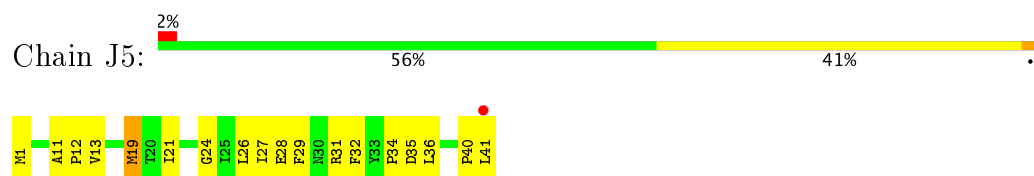
- Molecule 8: Photosystem I reaction center subunit IX



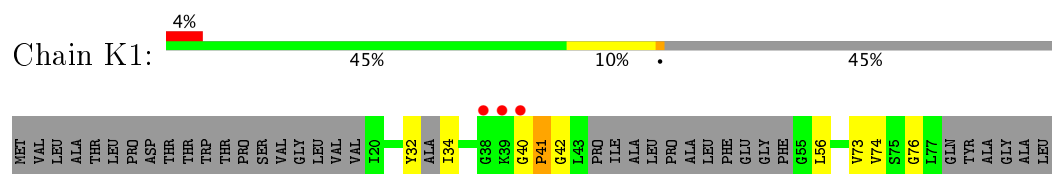
- Molecule 8: Photosystem I reaction center subunit IX



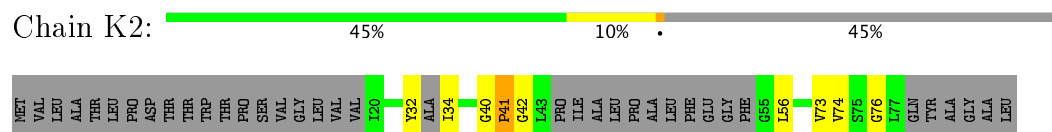
- Molecule 8: Photosystem I reaction center subunit IX



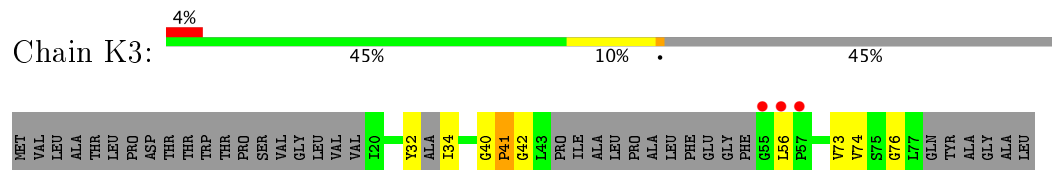
- Molecule 9: Photosystem I reaction center subunit Psak



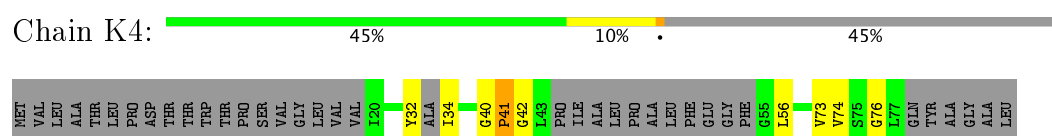
- Molecule 9: Photosystem I reaction center subunit Psak



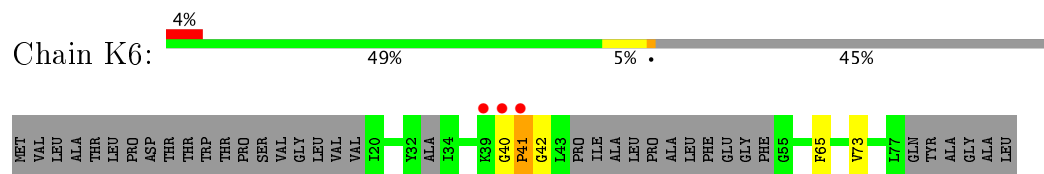
- Molecule 9: Photosystem I reaction center subunit PsaK



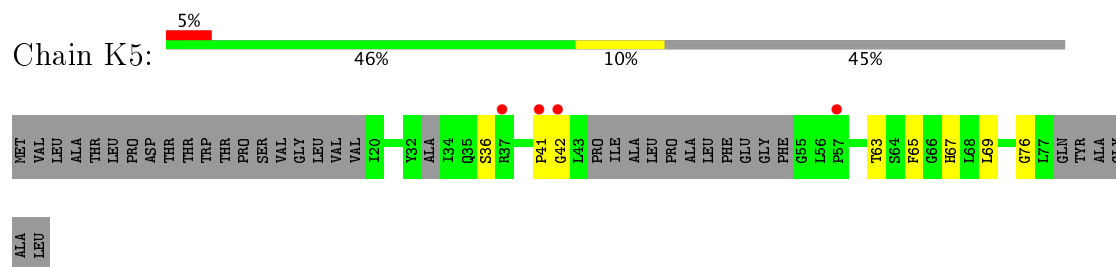
- Molecule 9: Photosystem I reaction center subunit PsaK



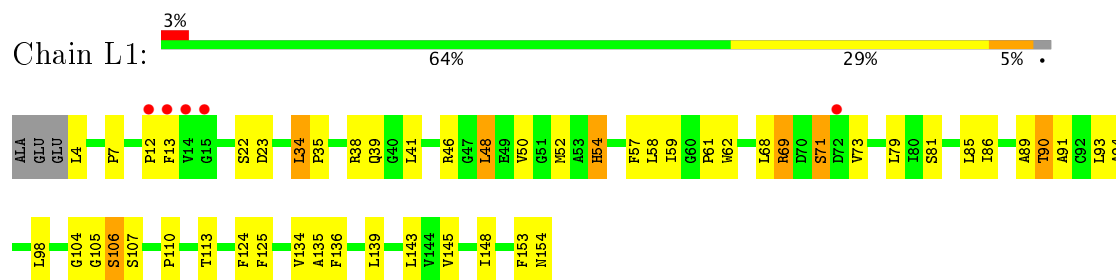
- Molecule 9: Photosystem I reaction center subunit PsaK



- Molecule 9: Photosystem I reaction center subunit PsaK

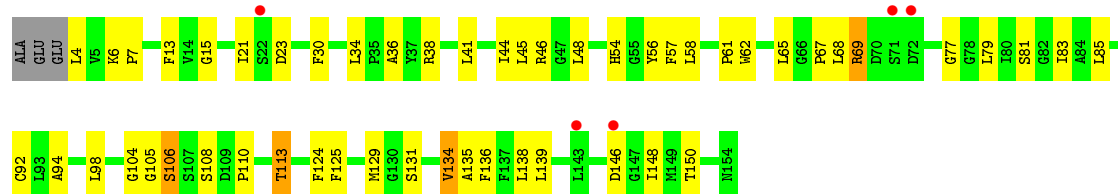


- Molecule 10: Photosystem I reaction center subunit XI

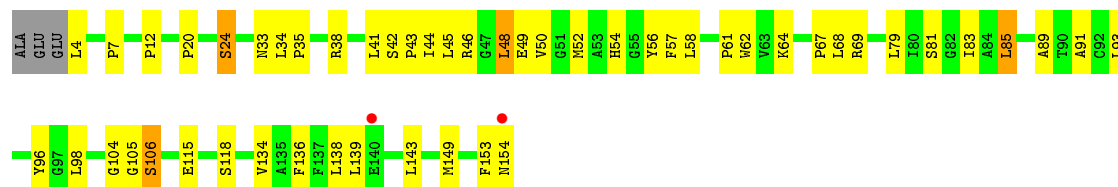


- Molecule 10: Photosystem I reaction center subunit XI

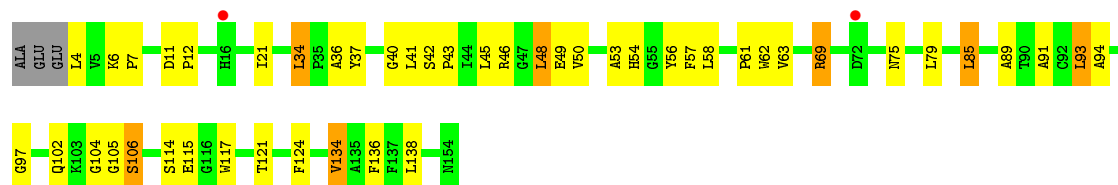




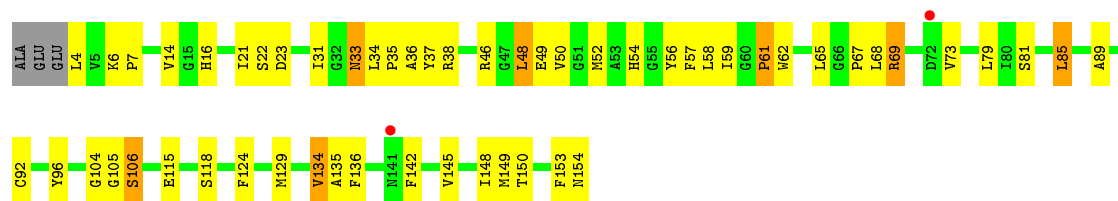
• Molecule 10: Photosystem I reaction center subunit XI



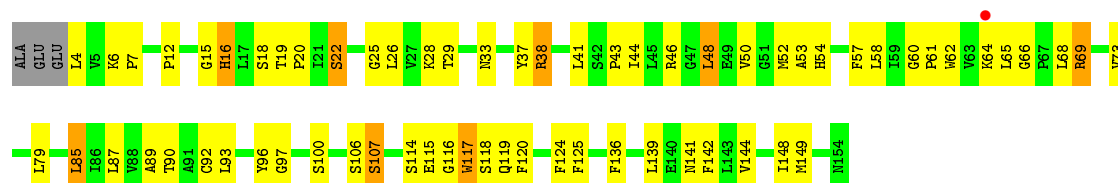
• Molecule 10: Photosystem I reaction center subunit XI



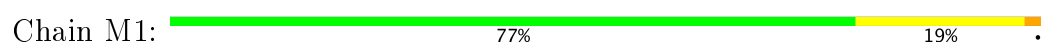
• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 11: Photosystem I reaction center subunit XII





- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



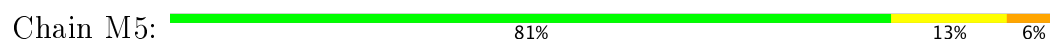
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Psax

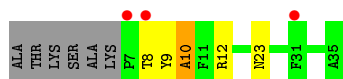


- Molecule 12: Psax

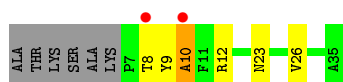




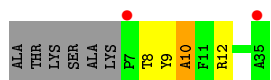
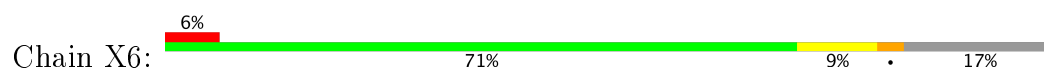
• Molecule 12: PsaX



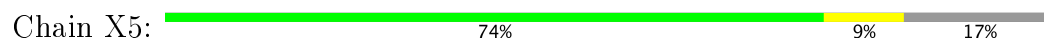
• Molecule 12: PsaX



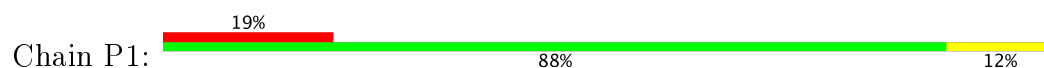
• Molecule 12: PsaX



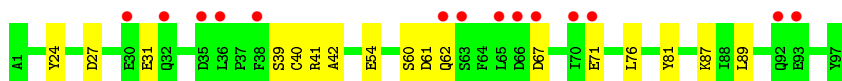
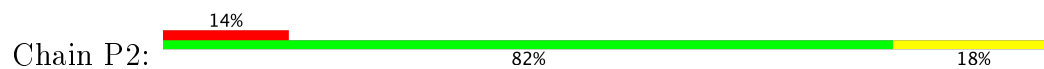
• Molecule 12: PsaX



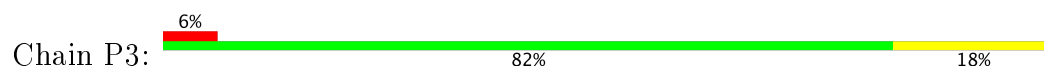
• Molecule 13: Ferredoxin-1

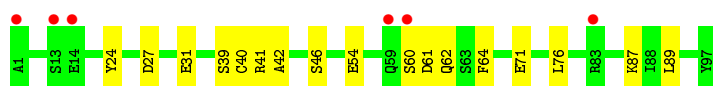


• Molecule 13: Ferredoxin-1

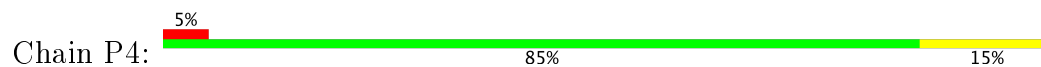


• Molecule 13: Ferredoxin-1

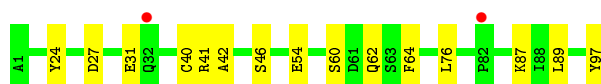
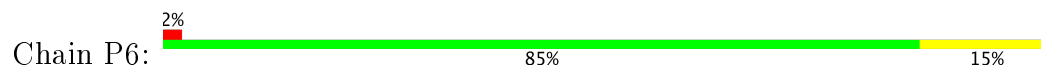




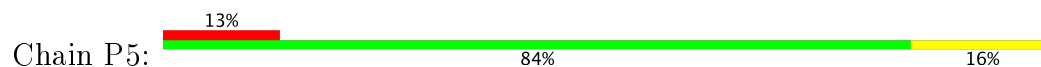
- Molecule 13: Ferredoxin-1



- Molecule 13: Ferredoxin-1



- Molecule 13: Ferredoxin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	214.10Å 239.67Å 265.61Å 90.00° 101.08° 90.00°	Depositor
Resolution (Å)	158.04 – 4.20 144.70 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (158.04-4.20) 99.9 (144.70-4.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 4.15Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.353 , 0.377 0.358 , 0.379	Depositor DCC
R_{free} test set	9617 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 73.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	148494	wwPDB-VP
Average B, all atoms (Å ²)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A1	0.39	0/5983	0.63	1/8158 (0.0%)
1	A2	0.40	0/5983	0.64	1/8158 (0.0%)
1	A3	0.40	0/5983	0.65	1/8158 (0.0%)
1	A4	0.41	0/5983	0.66	2/8158 (0.0%)
1	A5	0.39	0/5983	0.64	1/8158 (0.0%)
1	A6	0.42	0/5983	0.67	1/8158 (0.0%)
2	B1	0.40	0/6096	0.62	0/8332
2	B2	0.39	0/6096	0.63	0/8332
2	B3	0.39	0/6096	0.63	1/8332 (0.0%)
2	B4	0.43	0/6096	0.68	1/8332 (0.0%)
2	B5	0.40	0/6096	0.63	1/8332 (0.0%)
2	B6	0.43	0/6096	0.65	1/8332 (0.0%)
3	C1	0.43	0/608	0.69	0/824
3	C2	0.46	0/608	0.79	0/824
3	C3	0.49	0/608	0.78	0/824
3	C4	0.51	0/608	0.83	3/824 (0.4%)
3	C5	0.45	0/608	0.84	0/824
3	C6	0.49	0/608	0.82	3/824 (0.4%)
4	D1	0.39	0/1101	0.63	0/1492
4	D2	0.40	0/1101	0.71	1/1492 (0.1%)
4	D3	0.46	0/1101	0.75	1/1492 (0.1%)
4	D4	0.45	0/1101	0.75	1/1492 (0.1%)
4	D5	0.39	0/1101	0.60	0/1492
4	D6	0.46	0/1101	0.74	1/1492 (0.1%)
5	E1	0.43	0/551	0.67	0/750
5	E2	0.44	0/551	0.70	0/750
5	E3	0.50	0/551	0.69	0/750
5	E4	0.48	0/551	0.69	0/750
5	E5	0.41	0/551	0.57	0/750
5	E6	0.42	0/551	0.68	0/750
6	F1	0.37	0/1087	0.62	0/1476
6	F2	0.36	0/1087	0.62	0/1476

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	F3	0.38	0/1087	0.63	0/1476
6	F4	0.39	0/1087	0.66	0/1476
6	F5	0.37	0/1087	0.56	0/1476
6	F6	0.36	0/1087	0.58	0/1476
7	I1	0.47	0/312	0.67	0/425
7	I2	0.42	0/312	0.70	0/425
7	I3	0.49	0/312	0.75	0/425
7	I4	0.50	0/312	0.77	0/425
7	I5	0.42	0/312	0.65	0/425
7	I6	0.43	0/312	0.60	0/425
8	J1	0.38	0/350	0.53	0/477
8	J2	0.37	0/350	0.60	0/477
8	J3	0.39	0/350	0.60	0/477
8	J4	0.39	0/350	0.63	0/477
8	J5	0.39	0/350	0.49	0/477
8	J6	0.38	0/350	0.55	0/477
9	K1	0.39	0/219	0.60	0/297
9	K2	0.34	0/219	0.61	0/297
9	K3	0.36	0/219	0.67	0/297
9	K4	0.36	0/219	0.65	0/297
9	K5	0.42	0/219	0.55	0/297
9	K6	0.38	0/219	0.55	0/297
10	L1	0.41	0/1148	0.67	0/1558
10	L2	0.40	0/1148	0.69	0/1558
10	L3	0.46	0/1148	0.72	0/1558
10	L4	0.47	0/1148	0.72	0/1558
10	L5	0.44	0/1148	0.62	0/1558
10	L6	0.43	0/1148	0.69	0/1558
11	M1	0.43	0/244	0.73	0/332
11	M2	0.45	0/244	0.72	0/332
11	M3	0.47	0/244	0.72	1/332 (0.3%)
11	M4	0.50	0/244	0.69	0/332
11	M5	0.45	0/244	0.69	0/332
11	M6	0.42	0/244	0.68	0/332
12	X1	0.37	0/242	0.55	0/332
12	X2	0.40	0/242	0.57	0/332
12	X3	0.38	0/242	0.57	0/332
12	X4	0.37	0/242	0.58	0/332
12	X5	0.39	0/242	0.46	0/332
12	X6	0.36	0/242	0.55	0/332
13	P1	0.46	0/758	0.73	1/1029 (0.1%)
13	P2	0.46	0/758	0.73	1/1029 (0.1%)
13	P3	0.46	0/758	0.73	1/1029 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
13	P4	0.46	0/758	0.73	1/1029 (0.1%)
13	P5	0.47	0/758	0.73	1/1029 (0.1%)
13	P6	0.46	0/758	0.73	1/1029 (0.1%)
All	All	0.41	0/112194	0.66	28/152892 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C1	0	1
3	C5	0	4
All	All	0	5

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D4	131	THR	N-CA-C	-6.86	92.48	111.00
4	D6	131	THR	N-CA-C	-6.73	92.83	111.00
4	D3	131	THR	N-CA-C	-6.71	92.88	111.00
4	D2	131	THR	N-CA-C	-6.33	93.92	111.00
2	B6	260	PHE	CB-CA-C	-6.27	97.86	110.40
2	B4	260	PHE	CB-CA-C	-6.16	98.08	110.40
11	M3	30	TYR	N-CA-C	5.81	126.69	111.00
3	C4	60	ASP	CA-C-N	-5.78	104.49	117.20
2	B5	651	VAL	CB-CA-C	-5.70	100.58	111.40
3	C6	60	ASP	CA-C-N	-5.68	104.69	117.20
1	A6	521	GLY	N-CA-C	-5.67	98.91	113.10
1	A4	521	GLY	N-CA-C	-5.63	99.03	113.10
2	B3	260	PHE	CB-CA-C	-5.38	99.64	110.40
3	C4	60	ASP	O-C-N	5.33	131.22	122.70
3	C6	60	ASP	O-C-N	5.27	131.13	122.70
1	A1	521	GLY	N-CA-C	-5.22	100.06	113.10
1	A5	521	GLY	N-CA-C	-5.21	100.07	113.10
1	A3	521	GLY	N-CA-C	-5.21	100.08	113.10
3	C6	61	PHE	N-CA-CB	5.21	119.97	110.60
1	A2	521	GLY	N-CA-C	-5.20	100.10	113.10
13	P1	89	LEU	CA-CB-CG	5.20	127.25	115.30
13	P5	89	LEU	CA-CB-CG	5.19	127.23	115.30
13	P6	89	LEU	CA-CB-CG	5.19	127.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P3	89	LEU	CA-CB-CG	5.17	127.20	115.30
13	P4	89	LEU	CA-CB-CG	5.16	127.16	115.30
3	C4	61	PHE	N-CA-CB	5.13	119.84	110.60
13	P2	89	LEU	CA-CB-CG	5.12	127.08	115.30
1	A4	114	ALA	N-CA-C	-5.06	97.35	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C1	61	PHE	Peptide
3	C5	14	THR	Peptide
3	C5	15	GLN	Peptide
3	C5	40	SER	Peptide
3	C5	60	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	5784	0	5641	277	0
1	A2	5784	0	5638	248	0
1	A3	5784	0	5641	228	0
1	A4	5784	0	5639	243	0
1	A5	5784	0	5637	228	0
1	A6	5784	0	5641	214	0
2	B1	5879	0	5634	469	0
2	B2	5879	0	5633	278	0
2	B3	5879	0	5634	317	0
2	B4	5879	0	5633	326	0
2	B5	5879	0	5634	292	0
2	B6	5879	0	5633	262	0
3	C1	598	0	586	33	0
3	C2	598	0	586	36	0
3	C3	598	0	587	34	0
3	C4	598	0	584	34	0
3	C5	598	0	586	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C6	598	0	584	30	0
4	D1	1075	0	1077	18	0
4	D2	1075	0	1077	21	0
4	D3	1075	0	1077	20	0
4	D4	1075	0	1077	25	0
4	D5	1075	0	1077	13	0
4	D6	1075	0	1077	20	0
5	E1	539	0	528	7	0
5	E2	539	0	528	34	0
5	E3	539	0	528	21	0
5	E4	539	0	528	27	0
5	E5	539	0	528	12	0
5	E6	539	0	528	18	0
6	F1	1065	0	1077	24	0
6	F2	1065	0	1077	39	0
6	F3	1065	0	1077	21	0
6	F4	1065	0	1077	32	0
6	F5	1065	0	1077	21	0
6	F6	1065	0	1077	33	0
7	I1	301	0	306	29	0
7	I2	301	0	306	24	0
7	I3	301	0	306	15	0
7	I4	301	0	306	31	0
7	I5	301	0	306	19	0
7	I6	301	0	306	13	0
8	J1	338	0	347	22	0
8	J2	338	0	347	16	0
8	J3	338	0	347	19	0
8	J4	338	0	347	26	0
8	J5	338	0	347	25	0
8	J6	338	0	347	26	0
9	K1	222	0	110	7	0
9	K2	222	0	110	6	0
9	K3	222	0	110	4	0
9	K4	222	0	110	6	0
9	K5	222	0	110	2	0
9	K6	222	0	110	4	0
10	L1	1119	0	1125	45	0
10	L2	1119	0	1125	53	0
10	L3	1119	0	1125	64	0
10	L4	1119	0	1125	54	0
10	L5	1119	0	1125	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L6	1119	0	1125	60	0
11	M1	241	0	264	5	0
11	M2	241	0	264	8	0
11	M3	241	0	264	21	0
11	M4	241	0	264	17	0
11	M5	241	0	264	6	0
11	M6	241	0	264	9	0
12	X1	233	0	231	6	0
12	X2	233	0	231	10	0
12	X3	233	0	231	8	0
12	X4	233	0	231	19	0
12	X5	233	0	231	0	0
12	X6	233	0	231	4	0
13	P1	748	0	705	37	0
13	P2	748	0	705	53	0
13	P3	748	0	705	34	0
13	P4	748	0	705	44	0
13	P5	748	0	705	33	0
13	P6	748	0	705	23	0
14	A1	2310	0	2272	156	0
14	A2	2615	0	2593	177	0
14	A3	2622	0	2603	179	0
14	A4	2485	0	2449	155	0
14	A5	2516	0	2502	154	0
14	A6	2420	0	2377	168	0
14	B1	2477	0	2443	439	0
14	B2	2295	0	2256	233	0
14	B3	2466	0	2419	302	0
14	B4	2531	0	2491	273	0
14	B5	2466	0	2419	242	0
14	B6	2295	0	2256	210	0
14	F1	45	0	33	1	0
14	F2	82	0	58	13	0
14	F3	45	0	33	3	0
14	F4	45	0	33	7	0
14	F5	45	0	33	4	0
14	F6	45	0	33	14	0
14	I1	65	0	72	3	0
14	I6	65	0	72	2	0
14	J1	82	0	58	12	0
14	J2	45	0	33	6	0
14	J3	82	0	58	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	J4	82	0	58	12	0
14	J5	82	0	58	9	0
14	J6	147	0	130	7	0
14	K1	45	0	33	4	0
14	K2	45	0	33	3	0
14	K3	45	0	33	1	0
14	K4	45	0	33	3	0
14	K5	86	0	62	1	0
14	K6	45	0	33	2	0
14	L1	325	0	360	25	0
14	L2	260	0	288	23	0
14	L3	240	0	249	32	0
14	L4	260	0	288	38	0
14	L5	305	0	321	41	0
14	L6	325	0	360	47	0
14	M1	54	0	48	3	0
14	M2	54	0	48	1	0
14	M3	45	0	33	11	0
14	M6	54	0	48	2	0
14	X1	45	0	33	2	0
14	X2	45	0	33	6	0
14	X3	45	0	33	1	0
14	X4	45	0	33	16	0
14	X5	45	0	33	2	0
14	X6	45	0	33	1	0
15	A1	33	0	46	3	0
15	A2	33	0	46	3	0
15	A3	33	0	46	2	0
15	A4	33	0	46	2	0
15	A5	33	0	46	2	0
15	A6	33	0	46	4	0
15	B1	33	0	46	5	0
15	B2	33	0	46	1	0
15	B3	33	0	46	3	0
15	B4	33	0	46	7	0
15	B5	33	0	46	2	0
15	B6	33	0	46	1	0
16	A1	240	0	336	33	0
16	A2	240	0	336	20	0
16	A3	280	0	392	27	0
16	A4	240	0	336	23	0
16	A5	280	0	392	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A6	280	0	392	28	0
16	B1	305	0	425	32	0
16	B2	265	0	369	20	0
16	B3	225	0	313	25	0
16	B4	225	0	313	23	0
16	B5	225	0	313	18	0
16	B6	225	0	313	17	0
16	F1	40	0	56	2	0
16	F2	80	0	112	5	0
16	F3	80	0	112	3	0
16	F4	120	0	168	15	0
16	F5	40	0	56	2	0
16	F6	80	0	112	3	0
16	I1	80	0	112	12	0
16	I2	40	0	56	5	0
16	I3	80	0	112	7	0
16	I4	80	0	112	12	0
16	I5	80	0	112	5	0
16	I6	40	0	56	3	0
16	J1	80	0	112	13	0
16	J2	80	0	112	10	0
16	J3	80	0	112	6	0
16	J4	80	0	112	13	0
16	J5	120	0	168	22	0
16	J6	80	0	112	14	0
16	L1	80	0	112	12	0
16	L2	120	0	168	10	0
16	L3	80	0	112	9	0
16	L4	80	0	112	13	0
16	L5	80	0	112	11	0
16	L6	120	0	168	9	0
16	M1	40	0	56	2	0
16	M2	40	0	56	2	0
16	M3	40	0	56	9	0
16	M4	40	0	56	6	0
16	M5	40	0	56	3	0
16	M6	40	0	56	2	0
17	A1	76	0	98	6	0
17	A2	76	0	98	5	0
17	A3	76	0	98	5	0
17	A4	76	0	98	7	0
17	A5	76	0	98	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	A6	76	0	98	5	0
17	B1	23	0	16	2	0
17	B2	23	0	16	2	0
17	B6	23	0	16	2	0
17	X3	23	0	16	6	0
17	X4	23	0	16	1	0
17	X5	23	0	16	0	0
18	A1	8	0	0	6	0
18	A2	8	0	0	4	0
18	A3	8	0	0	8	0
18	A4	8	0	0	4	0
18	A5	8	0	0	5	0
18	B6	8	0	0	7	0
18	C1	16	0	0	12	0
18	C2	16	0	0	13	0
18	C3	16	0	0	12	0
18	C4	16	0	0	7	0
18	C5	16	0	0	13	0
18	C6	16	0	0	8	0
19	B1	55	0	86	8	0
19	B2	55	0	86	6	0
19	B3	55	0	86	8	0
19	B4	55	0	86	8	0
19	B5	55	0	86	9	0
19	B6	55	0	86	10	0
20	L1	2	0	0	0	0
20	L2	1	0	0	0	0
20	L4	2	0	0	0	0
20	L6	1	0	0	0	0
21	P1	4	0	0	0	0
21	P2	4	0	0	0	0
21	P3	4	0	0	0	0
21	P4	4	0	0	0	0
21	P5	4	0	0	0	0
21	P6	4	0	0	0	0
All	All	148494	0	147087	5478	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (5478) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:40:ARG:CG	13:P5:60:SER:HB2	1.30	1.60
1:A5:40:ARG:HG3	13:P5:60:SER:CB	1.37	1.52
1:A5:40:ARG:CG	13:P5:60:SER:CB	1.84	1.51
1:A1:36:ARG:NH1	13:P1:70:ILE:HG13	1.18	1.43
5:E5:39:ARG:NH1	13:P5:24:TYR:CZ	1.89	1.37
1:A1:36:ARG:NH1	13:P1:70:ILE:CG1	1.92	1.33
5:E5:39:ARG:NH1	13:P5:24:TYR:CE2	1.99	1.30
5:E4:39:ARG:NH1	13:P4:24:TYR:OH	1.65	1.29
1:A1:40:ARG:HG2	13:P1:61:ASP:OD1	1.12	1.28
1:A4:578:CYS:SG	18:A4:852:SF4:FE3	1.25	1.26
5:E5:39:ARG:CZ	13:P5:24:TYR:OH	1.84	1.25
1:A5:36:ARG:NH1	13:P5:67:ASP:O	1.70	1.23
1:A5:40:ARG:HG2	13:P5:60:SER:OG	1.34	1.23
2:B1:531:LEU:HD11	14:B1:802:CLA:O1A	1.38	1.23
1:A2:36:ARG:NH1	13:P2:67:ASP:O	1.75	1.20
5:E4:57:THR:HG23	13:P4:42:ALA:CB	1.72	1.19
5:E2:3:ARG:NH2	13:P2:31:GLU:OE1	1.75	1.19
5:E4:37:ILE:HD13	13:P4:41:ARG:HD3	1.22	1.17
2:B1:25:ALA:HB2	19:B1:850:LMG:H121	1.23	1.17
2:B1:622:LEU:HD12	14:B1:805:CLA:C1	1.74	1.15
5:E4:57:THR:HG23	13:P4:42:ALA:HB2	1.15	1.15
3:C2:20:CYS:SG	18:C2:101:SF4:FE2	1.38	1.14
5:E4:57:THR:HG21	13:P4:42:ALA:HA	1.28	1.14
5:E6:37:ILE:HD13	13:P6:41:ARG:HD3	1.30	1.14
2:B3:21:TRP:CZ2	14:B3:1842:CLA:HMB1	1.84	1.12
2:B4:622:LEU:HD12	14:B4:804:CLA:C1	1.79	1.12
1:A5:40:ARG:HG2	13:P5:60:SER:CB	1.62	1.11
5:E5:39:ARG:CZ	13:P5:24:TYR:CZ	2.34	1.11
10:L4:134:VAL:HG23	16:L4:208:BCR:H403	1.31	1.10
1:A4:40:ARG:CG	13:P4:60:SER:O	1.99	1.10
5:E4:39:ARG:CZ	13:P4:24:TYR:OH	1.99	1.10
5:E4:39:ARG:NH1	13:P4:24:TYR:CZ	2.18	1.10
9:K6:73:VAL:HA	14:K6:1401:CLA:HBB1	1.34	1.09
5:E2:3:ARG:HH22	13:P2:31:GLU:CG	1.65	1.09
2:B2:425:LEU:HG	14:B2:838:CLA:CBB	1.82	1.09
1:A6:587:CYS:SG	18:B6:801:SF4:FE2	1.43	1.09
1:A4:36:ARG:HD2	13:P4:67:ASP:OD1	1.50	1.08
5:E4:57:THR:CG2	13:P4:42:ALA:CB	2.31	1.08
1:A1:39:ALA:HB1	13:P1:60:SER:HB2	1.19	1.07
14:B1:854:CLA:H91	14:L2:207:CLA:H93	1.35	1.07
2:B1:622:LEU:HD12	14:B1:805:CLA:H11	1.16	1.07
5:E3:3:ARG:HH12	13:P3:31:GLU:HB2	1.20	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K1:73:VAL:HA	14:K1:1401:CLA:HBB1	1.34	1.07
1:A1:40:ARG:CG	13:P1:61:ASP:OD1	2.02	1.07
2:B2:229:TRP:HB2	14:B2:815:CLA:H12	1.34	1.07
5:E2:39:ARG:NH1	13:P2:24:TYR:CE2	2.23	1.07
5:E2:3:ARG:HH22	13:P2:31:GLU:CB	1.67	1.06
1:A1:36:ARG:HH22	13:P1:70:ILE:HB	1.20	1.06
9:K2:73:VAL:HA	14:K2:1401:CLA:HBB1	1.13	1.05
2:B3:166:TRP:CZ2	14:B3:1813:CLA:HMA1	1.90	1.05
2:B1:298:HIS:CE1	14:B1:823:CLA:OBD	2.10	1.05
2:B2:425:LEU:HG	14:B2:838:CLA:HBB1	1.32	1.05
2:B6:425:LEU:HG	14:B6:839:CLA:CBB	1.87	1.05
5:E4:37:ILE:HD13	13:P4:41:ARG:CD	1.87	1.04
14:B1:854:CLA:HMB3	7:I1:20:TRP:CZ2	1.91	1.04
2:B1:52:HIS:CE1	14:B1:807:CLA:CMA	2.39	1.04
8:J5:31:ARG:HD3	16:J5:104:BCR:H312	1.38	1.04
7:I4:20:TRP:NE1	16:I4:102:BCR:HC22	1.72	1.03
1:A3:40:ARG:HD3	13:P3:60:SER:O	1.58	1.03
1:A1:40:ARG:CD	13:P1:61:ASP:HA	1.89	1.03
2:B6:122:TRP:CZ2	14:B6:813:CLA:H191	1.94	1.02
10:L6:142:PHE:CE1	14:L6:208:CLA:H12	1.93	1.02
5:E3:37:ILE:HD13	13:P3:41:ARG:CD	1.88	1.02
14:B4:812:CLA:H91	14:L6:208:CLA:H93	1.38	1.02
2:B4:622:LEU:HD12	14:B4:804:CLA:H11	1.02	1.02
10:L3:61:PRO:HB3	14:L3:205:CLA:HBB1	1.41	1.02
1:A4:578:CYS:SG	18:A4:852:SF4:S4	2.58	1.01
6:F6:76:TRP:NE1	14:F6:202:CLA:HBD	1.75	1.01
14:B1:854:CLA:HMB3	7:I1:20:TRP:HZ2	1.22	1.01
5:E5:39:ARG:NH2	13:P5:24:TYR:OH	1.94	1.01
1:A5:36:ARG:NH1	13:P5:70:ILE:HB	1.76	1.00
2:B2:339:TRP:HE1	14:B2:823:CLA:C2B	1.72	1.00
8:J1:24:GLY:HA3	14:J1:101:CLA:HBB1	1.42	1.00
2:B1:122:TRP:CZ2	14:B1:814:CLA:H201	1.95	1.00
12:X4:26:VAL:HB	14:X4:102:CLA:HED1	1.44	1.00
1:A5:36:ARG:HH11	13:P5:70:ILE:HB	1.23	1.00
1:A2:578:CYS:SG	18:A2:1655:SF4:S4	2.60	1.00
1:A1:39:ALA:CB	13:P1:60:SER:HB2	1.92	0.99
1:A3:270:PHE:CE1	14:A3:844:CLA:HMD2	1.97	0.99
1:A4:536:PHE:HA	14:A4:836:CLA:HED1	1.45	0.99
3:C5:13:CYS:SG	3:C5:15:GLN:HB2	2.02	0.99
1:A5:313:HIS:CE1	16:A5:845:BCR:H363	1.98	0.98
2:B3:48:SER:OG	14:B3:1807:CLA:HBB1	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:278:ALA:HB2	14:B1:818:CLA:HBB1	1.44	0.98
3:C3:47:CYS:SG	18:C3:101:SF4:FE4	1.55	0.98
3:C3:50:CYS:HG	18:C3:101:SF4:FE1	0.71	0.97
3:C1:20:CYS:SG	18:C1:101:SF4:FE2	1.56	0.97
1:A1:36:ARG:NH2	13:P1:70:ILE:HB	1.79	0.97
1:A2:536:PHE:HA	14:A2:1639:CLA:HED1	1.46	0.97
1:A5:536:PHE:HA	14:A5:837:CLA:HED1	1.44	0.97
5:E2:3:ARG:HH22	13:P2:31:GLU:HB2	1.27	0.97
2:B1:342:ALA:HB2	16:B1:847:BCR:H372	1.47	0.97
2:B4:622:LEU:CD1	14:B4:804:CLA:H11	1.95	0.96
10:L4:62:TRP:CZ2	14:L4:201:CLA:H11	2.00	0.96
18:A5:854:SF4:FE1	2:B5:574:CYS:SG	1.56	0.96
2:B1:52:HIS:CE1	14:B1:807:CLA:HMA1	1.98	0.96
3:C5:20:CYS:HG	18:C5:101:SF4:FE2	0.70	0.96
18:A1:850:SF4:FE4	2:B1:565:CYS:HG	0.80	0.96
1:A1:578:CYS:SG	18:A1:850:SF4:FE3	1.56	0.96
2:B5:153:TRP:CZ3	14:B5:1801:CLA:H62	1.99	0.96
3:C1:47:CYS:HG	18:C1:101:SF4:FE4	0.83	0.96
2:B6:229:TRP:HB2	14:B6:816:CLA:H12	1.47	0.96
3:C6:20:CYS:HG	18:C6:101:SF4:FE2	0.83	0.96
2:B5:630:LEU:HD22	14:B5:1803:CLA:HMD1	1.45	0.96
2:B1:525:VAL:HG12	14:B1:804:CLA:H141	1.45	0.96
2:B6:574:CYS:HG	18:B6:801:SF4:FE1	0.80	0.96
2:B1:122:TRP:HZ2	14:B1:814:CLA:H191	1.30	0.95
3:C6:50:CYS:HG	18:C6:101:SF4:FE1	0.69	0.95
5:E2:3:ARG:NH2	13:P2:31:GLU:HB2	1.80	0.95
3:C5:47:CYS:HG	18:C5:101:SF4:FE4	0.75	0.95
11:M3:9:TYR:HB3	16:M3:1602:BCR:H401	1.48	0.95
1:A1:36:ARG:CZ	13:P1:70:ILE:HG13	1.96	0.95
1:A5:36:ARG:HH12	13:P5:71:GLU:H	1.12	0.95
2:B6:340:HIS:CD2	14:B6:824:CLA:HAA1	2.01	0.95
2:B1:229:TRP:HB2	14:B1:817:CLA:H12	1.48	0.94
2:B4:256:PHE:CE1	14:B4:819:CLA:HAB	2.02	0.94
16:L6:201:BCR:H313	14:L6:202:CLA:H143	1.48	0.94
1:A1:36:ARG:HH12	13:P1:70:ILE:CG1	1.68	0.94
1:A1:536:PHE:HA	14:A1:835:CLA:HED1	1.48	0.94
1:A5:40:ARG:HG3	13:P5:60:SER:CA	1.96	0.94
3:C3:13:CYS:HG	18:C3:102:SF4:FE3	0.74	0.94
3:C1:10:CYS:SG	18:C1:102:SF4:FE4	1.60	0.94
1:A3:40:ARG:CD	13:P3:60:SER:O	2.14	0.94
3:C5:10:CYS:HG	18:C5:102:SF4:FE4	0.63	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E4:57:THR:HG21	13:P4:42:ALA:CA	1.97	0.93
2:B4:189:TRP:CA	14:B4:816:CLA:HBB1	1.98	0.93
2:B4:189:TRP:HA	14:B4:816:CLA:HBB1	1.51	0.93
2:B3:622:LEU:HD12	14:B3:1804:CLA:H11	1.51	0.93
2:B1:622:LEU:CD1	14:B1:805:CLA:H11	1.99	0.93
1:A6:536:PHE:HA	14:A6:1637:CLA:HED1	1.50	0.93
3:C5:61:PHE:O	3:C5:62:LEU:O	1.87	0.93
18:A2:1655:SF4:FE1	2:B2:574:CYS:HG	0.66	0.92
1:A3:578:CYS:SG	18:A3:855:SF4:FE3	1.61	0.92
2:B2:438:GLY:HA3	14:B2:832:CLA:CBB	1.99	0.92
1:A3:536:PHE:HA	14:A3:838:CLA:HED1	1.50	0.92
2:B5:630:LEU:HD22	14:B5:1803:CLA:CMD	1.98	0.92
2:B3:425:LEU:HG	14:B3:1841:CLA:CBB	1.98	0.92
2:B3:256:PHE:CE1	14:B3:1819:CLA:HAB	2.05	0.92
2:B1:229:TRP:C	14:B1:817:CLA:HBA2	1.90	0.92
2:B1:531:LEU:CD1	14:B1:802:CLA:O1A	2.17	0.92
5:E5:39:ARG:NH2	13:P5:81:TYR:OH	2.02	0.92
3:C2:13:CYS:SG	18:C2:102:SF4:FE3	1.61	0.92
2:B1:230:GLY:HA2	14:B1:817:CLA:HAA2	1.51	0.92
10:L5:53:ALA:CB	14:L5:205:CLA:HED3	2.00	0.92
2:B3:21:TRP:HZ2	14:B3:1842:CLA:HMB1	1.31	0.92
3:C4:57:CYS:HG	18:C4:102:SF4:FE1	0.63	0.91
2:B1:493:PRO:HG3	14:B1:837:CLA:C1D	2.00	0.91
14:B1:811:CLA:H203	7:I1:26:VAL:CG2	2.00	0.91
18:A5:854:SF4:FE1	2:B5:574:CYS:HG	0.78	0.91
2:B1:25:ALA:CB	19:B1:850:LMG:H121	1.99	0.91
14:L4:203:CLA:HBA2	16:L4:208:BCR:H363	1.52	0.91
1:A3:506:ALA:O	1:A6:627:PRO:HB3	1.71	0.91
3:C4:20:CYS:HG	18:C4:101:SF4:FE2	0.64	0.91
2:B1:52:HIS:CE1	14:B1:807:CLA:HMA2	2.04	0.91
2:B1:177:HIS:ND1	14:B1:825:CLA:O1D	2.03	0.91
8:J6:31:ARG:HD3	16:J6:1105:BCR:H312	1.51	0.91
2:B4:668:MET:SD	14:B4:805:CLA:MG	1.52	0.91
5:E6:37:ILE:CD1	13:P6:41:ARG:HD3	2.00	0.91
3:C3:11:ILE:HD12	13:P3:39:SER:O	1.71	0.91
3:C1:16:CYS:HG	18:C1:102:SF4:FE2	0.65	0.90
2:B6:64:LEU:HD11	16:B6:845:BCR:H271	1.53	0.90
2:B4:425:LEU:HG	14:B4:841:CLA:CBB	2.00	0.90
1:A4:36:ARG:NH1	13:P4:67:ASP:O	2.04	0.90
6:F6:76:TRP:CH2	14:F6:202:CLA:O1A	2.24	0.90
16:A3:852:BCR:H362	14:B3:1804:CLA:H42	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C5:57:CYS:HG	18:C5:102:SF4:FE1	0.65	0.89
5:E4:57:THR:CG2	13:P4:42:ALA:HB2	1.95	0.89
16:A6:1648:BCR:H362	14:A6:1651:CLA:H42	1.54	0.89
3:C1:13:CYS:SG	18:C1:102:SF4:FE3	1.64	0.89
1:A3:578:CYS:HG	18:A3:855:SF4:FE3	0.63	0.89
18:A3:855:SF4:FE4	2:B3:565:CYS:HG	0.86	0.89
1:A4:36:ARG:HD2	13:P4:67:ASP:CG	1.93	0.89
3:C4:13:CYS:SG	18:C4:102:SF4:FE3	1.63	0.89
8:J5:24:GLY:HA3	14:J5:101:CLA:HBB1	1.54	0.89
12:X3:12:ARG:HB3	17:X3:101:LHG:HC5	1.55	0.89
11:M2:24:ARG:HH21	14:L3:202:CLA:HED2	1.38	0.88
2:B1:535:THR:HG23	14:B1:802:CLA:HBD	1.53	0.88
6:F2:69:LEU:HB2	14:F2:204:CLA:CBB	2.02	0.88
16:A4:849:BCR:H362	14:B4:804:CLA:H42	1.54	0.88
2:B4:25:ALA:HB2	19:B4:851:LMG:H121	1.55	0.88
14:A6:1651:CLA:H11	2:B6:622:LEU:HD12	1.53	0.88
3:C6:13:CYS:HG	18:C6:102:SF4:FE3	0.89	0.87
1:A6:352:TRP:CD1	14:A6:1625:CLA:H201	2.08	0.87
16:A5:850:BCR:H362	14:B5:1804:CLA:H42	1.56	0.87
3:C3:20:CYS:HG	18:C3:101:SF4:FE2	0.63	0.87
3:C5:40:SER:HB3	3:C5:41:SER:HA	1.56	0.87
1:A1:40:ARG:HD3	13:P1:61:ASP:HA	1.54	0.87
3:C3:11:ILE:HD11	13:P3:40:CYS:HA	1.54	0.87
16:A2:1652:BCR:H362	14:B2:802:CLA:H42	1.56	0.87
2:B2:339:TRP:HZ2	14:B2:823:CLA:HAB	1.40	0.87
2:B4:180:GLY:HA3	14:B4:815:CLA:HBB1	1.56	0.87
2:B5:622:LEU:HD12	14:B5:1804:CLA:H11	1.57	0.87
14:A4:831:CLA:H143	16:L4:208:BCR:H313	1.57	0.86
2:B4:176:HIS:CG	14:B4:815:CLA:HMC2	2.10	0.86
3:C2:57:CYS:HG	18:C2:102:SF4:FE1	0.58	0.86
10:L4:134:VAL:CG2	16:L4:208:BCR:H403	2.05	0.86
10:L6:89:ALA:HB2	14:L6:203:CLA:H141	1.57	0.86
10:L6:58:LEU:HD21	14:L6:203:CLA:H192	1.55	0.86
2:B1:60:VAL:CG2	14:B1:829:CLA:H11	2.05	0.86
2:B6:339:TRP:HE1	14:B6:824:CLA:C2B	1.87	0.86
16:A1:847:BCR:H362	14:B1:805:CLA:H42	1.56	0.86
3:C6:11:ILE:CD1	13:P6:40:CYS:HA	2.04	0.86
2:B2:60:VAL:CG2	14:B2:827:CLA:H11	2.05	0.86
5:E4:57:THR:CG2	13:P4:42:ALA:HA	2.04	0.86
6:F2:88:VAL:HG12	6:F2:94:ALA:HA	1.57	0.86
2:B6:438:GLY:HA3	14:B6:833:CLA:CBB	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:189:TRP:HA	14:B3:1816:CLA:HBB1	1.56	0.86
8:J4:24:GLY:HA3	14:J4:101:CLA:HBB1	1.57	0.86
1:A5:36:ARG:HH12	13:P5:71:GLU:N	1.72	0.86
2:B6:425:LEU:HG	14:B6:839:CLA:HBB1	1.58	0.85
10:L3:138:LEU:HD13	14:L3:205:CLA:H92	1.59	0.85
2:B6:339:TRP:HE1	14:B6:824:CLA:C3B	1.88	0.85
3:C5:47:CYS:SG	18:C5:101:SF4:FE4	1.68	0.85
3:C6:57:CYS:HG	18:C6:102:SF4:FE1	0.88	0.85
2:B3:725:LEU:HD11	14:B3:1831:CLA:H203	1.58	0.85
5:E3:37:ILE:HD13	13:P3:41:ARG:HD3	1.58	0.85
2:B1:28:HIS:ND1	14:B1:808:CLA:O1A	2.10	0.85
2:B1:53:LEU:CD1	14:B1:807:CLA:CGA	2.55	0.85
2:B1:427:TRP:HD1	14:B1:803:CLA:O1A	1.58	0.85
2:B1:230:GLY:N	14:B1:817:CLA:CBA	2.39	0.85
2:B1:466:ILE:CD1	14:B1:838:CLA:O2A	2.24	0.85
3:C3:57:CYS:HG	18:C3:102:SF4:FE1	0.91	0.85
2:B6:724:ILE:HD13	14:B6:827:CLA:HMC2	1.58	0.85
6:F4:73:ILE:HG23	14:F4:202:CLA:HAA1	1.59	0.85
11:M4:4:THR:N	11:M4:7:GLN:OE1	2.10	0.85
2:B1:173:ARG:HB3	14:B1:825:CLA:HMD1	1.59	0.84
2:B4:174:LEU:HD21	14:B4:826:CLA:C1D	2.06	0.84
2:B5:153:TRP:HZ3	14:B5:1801:CLA:H62	1.37	0.84
8:J1:27:ILE:CG2	16:J1:104:BCR:H343	2.06	0.84
9:K4:73:VAL:HA	14:K4:1401:CLA:HBB1	1.58	0.84
3:C6:11:ILE:HD12	13:P6:40:CYS:HA	1.59	0.84
1:A3:352:TRP:CD1	14:A3:825:CLA:H201	2.11	0.84
3:C5:50:CYS:HG	18:C5:101:SF4:FE1	0.92	0.84
9:K2:73:VAL:HA	14:K2:1401:CLA:CBB	2.03	0.84
1:A4:40:ARG:CD	13:P4:60:SER:O	2.25	0.84
2:B1:230:GLY:N	14:B1:817:CLA:HBA1	1.92	0.84
3:C6:15:GLN:OE1	13:P6:64:PHE:HE2	1.60	0.84
14:L1:201:CLA:H143	16:L1:209:BCR:H313	1.60	0.84
2:B3:176:HIS:CG	14:B3:1815:CLA:HMC2	2.11	0.84
8:J4:31:ARG:HD3	16:J4:104:BCR:H312	1.58	0.84
2:B1:313:LYS:O	2:B1:314:VAL:HG22	1.78	0.84
2:B3:65:PHE:CE2	14:B3:1809:CLA:CHD	2.60	0.84
2:B1:122:TRP:CZ2	14:B1:814:CLA:H191	2.13	0.84
2:B4:509:SER:O	2:B4:511:THR:N	2.11	0.83
12:X4:26:VAL:HG12	14:X4:102:CLA:CED	2.07	0.83
2:B4:176:HIS:ND1	14:B4:815:CLA:HMC2	1.94	0.83
1:A5:40:ARG:CB	13:P5:60:SER:HB2	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:207:GLY:C	14:B1:815:CLA:HMD1	1.98	0.83
2:B2:438:GLY:HA3	14:B2:832:CLA:HBB1	1.60	0.83
10:L3:48:LEU:HD13	14:L3:203:CLA:CED	2.08	0.83
2:B3:313:LYS:O	2:B3:314:VAL:HG22	1.77	0.83
18:A3:855:SF4:FE4	2:B3:565:CYS:SG	1.71	0.83
3:C3:13:CYS:SG	18:C3:102:SF4:FE3	1.68	0.83
14:A5:801:CLA:HBB1	14:B5:1804:CLA:HED1	1.61	0.83
5:E4:57:THR:CG2	13:P4:42:ALA:CA	2.55	0.83
2:B1:65:PHE:HE2	14:B1:809:CLA:CHD	1.91	0.83
2:B5:622:LEU:HD12	14:B5:1804:CLA:C1	2.08	0.83
14:L1:207:CLA:H93	14:B3:1812:CLA:H91	1.58	0.83
2:B6:438:GLY:HA3	14:B6:833:CLA:HBB1	1.60	0.83
2:B3:271:ASP:HB3	14:B3:1819:CLA:HMA1	1.60	0.83
1:A1:36:ARG:NH2	13:P1:70:ILE:CG2	2.42	0.83
2:B2:313:LYS:O	2:B2:314:VAL:HG22	1.79	0.82
1:A1:578:CYS:HG	18:A1:850:SF4:FE3	0.57	0.82
2:B3:430:LEU:HD13	14:B3:1802:CLA:HED3	1.59	0.82
5:E2:3:ARG:HH22	13:P2:31:GLU:CD	1.82	0.82
10:L5:115:GLU:O	10:L5:118:SER:OG	1.94	0.82
2:B1:274:HIS:HB3	14:B1:818:CLA:HMB3	1.60	0.82
2:B5:339:TRP:HE1	14:B5:1826:CLA:C2B	1.92	0.82
2:B5:525:VAL:HG12	14:B5:1803:CLA:H141	1.59	0.82
6:F3:88:VAL:HG12	6:F3:94:ALA:HA	1.62	0.82
8:J5:27:ILE:HD13	16:J5:104:BCR:C11	2.10	0.82
1:A3:180:TYR:OH	14:A3:811:CLA:O1D	1.97	0.82
3:C3:20:CYS:SG	18:C3:101:SF4:FE2	1.70	0.82
6:F1:88:VAL:HG12	6:F1:94:ALA:HA	1.62	0.82
1:A1:207:LEU:HD22	16:A1:843:BCR:H361	1.60	0.82
1:A4:203:GLY:HA2	14:A4:819:CLA:HBC1	1.60	0.82
8:J1:27:ILE:HD13	16:J1:104:BCR:C11	2.10	0.82
1:A1:36:ARG:HH11	13:P1:70:ILE:HG13	1.37	0.82
2:B6:278:ALA:HB2	14:B6:817:CLA:HBB1	1.61	0.82
5:E2:3:ARG:NH2	13:P2:31:GLU:CD	2.32	0.82
14:A2:1602:CLA:HBB1	14:B2:802:CLA:HED1	1.62	0.82
2:B1:122:TRP:CH2	14:B1:814:CLA:H201	2.15	0.81
2:B1:65:PHE:CE2	14:B1:809:CLA:CHD	2.62	0.81
1:A1:36:ARG:NH2	13:P1:70:ILE:CB	2.42	0.81
1:A5:281:PHE:CE1	14:A5:818:CLA:HAB	2.16	0.81
2:B3:509:SER:O	2:B3:511:THR:N	2.13	0.81
2:B3:189:TRP:CA	14:B3:1816:CLA:HBB1	2.09	0.81
2:B6:52:HIS:NE2	14:B6:806:CLA:HMA1	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:36:ARG:NH2	13:P3:71:GLU:OE2	2.13	0.81
1:A4:40:ARG:HG3	13:P4:60:SER:O	1.77	0.81
14:L4:205:CLA:H93	14:B5:1812:CLA:H91	1.62	0.81
2:B1:296:ILE:HG13	14:B1:822:CLA:OBD	1.81	0.81
2:B1:456:ILE:HD11	14:B1:834:CLA:CHB	2.11	0.81
2:B6:122:TRP:HZ2	14:B6:813:CLA:H191	1.41	0.81
3:C2:13:CYS:HG	18:C2:102:SF4:FE3	0.50	0.81
10:L3:49:GLU:OE2	14:L3:203:CLA:ND	2.13	0.81
3:C3:11:ILE:HD12	13:P3:39:SER:C	2.01	0.81
1:A3:612:HIS:ND1	14:A3:837:CLA:HMC2	1.96	0.81
2:B2:509:SER:O	2:B2:511:THR:N	2.13	0.81
2:B2:177:HIS:ND1	14:B2:823:CLA:O1D	2.13	0.81
2:B4:220:GLY:HA3	14:B4:817:CLA:HMD1	1.62	0.81
11:M3:21:LEU:HD21	14:M3:1601:CLA:HMA1	1.62	0.81
2:B1:45:ILE:HD12	14:B1:807:CLA:C2C	2.11	0.81
2:B5:509:SER:O	2:B5:511:THR:N	2.13	0.81
5:E3:3:ARG:NH1	13:P3:31:GLU:HB2	1.96	0.81
14:A2:1644:CLA:H192	10:L2:58:LEU:CD2	2.11	0.81
2:B5:725:LEU:HD11	14:B5:1831:CLA:H203	1.61	0.81
10:L3:49:GLU:OE2	14:L3:203:CLA:MG	1.21	0.81
14:A1:801:CLA:HBB1	14:B1:805:CLA:HED1	1.63	0.80
2:B3:390:PHE:CE1	16:B3:1849:BCR:H373	2.15	0.80
2:B6:313:LYS:O	2:B6:314:VAL:HG22	1.80	0.80
18:A1:850:SF4:FE4	2:B1:565:CYS:SG	1.71	0.80
2:B4:271:ASP:HB3	14:B4:819:CLA:HMA1	1.62	0.80
8:J3:31:ARG:HD3	16:J3:104:BCR:H312	1.62	0.80
1:A2:189:TRP:CZ2	14:A2:1615:CLA:HAC2	2.16	0.80
8:J2:24:GLY:HA3	14:J2:101:CLA:HBB1	1.63	0.80
2:B3:180:GLY:HA3	14:B3:1815:CLA:HBB1	1.62	0.80
10:L6:124:PHE:CE1	16:L6:209:BCR:H292	2.17	0.80
3:C1:47:CYS:SG	18:C1:101:SF4:FE4	1.74	0.80
1:A3:203:GLY:HA2	14:A3:820:CLA:HBC1	1.63	0.80
2:B1:509:SER:O	2:B1:511:THR:N	2.13	0.80
2:B5:313:LYS:O	2:B5:314:VAL:HG22	1.81	0.80
3:C1:16:CYS:SG	18:C1:102:SF4:FE2	1.74	0.80
12:X4:26:VAL:CG1	14:X4:102:CLA:CED	2.60	0.80
2:B1:25:ALA:HB2	19:B1:850:LMG:C12	2.07	0.80
2:B5:531:LEU:HD11	14:B5:1802:CLA:O1A	1.81	0.80
14:B2:809:CLA:H162	10:L3:56:TYR:OH	1.82	0.80
5:E6:39:ARG:CZ	13:P6:24:TYR:OH	2.30	0.80
6:F4:88:VAL:HG12	6:F4:94:ALA:HA	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J6:26:LEU:HD23	16:J6:1104:BCR:HC7	1.62	0.80
5:E2:3:ARG:NH2	13:P2:31:GLU:CG	2.43	0.80
14:A3:843:CLA:H151	10:L3:85:LEU:HD21	1.64	0.79
2:B4:525:VAL:HG12	14:B4:803:CLA:H141	1.63	0.79
2:B1:298:HIS:ND1	14:B1:823:CLA:OBD	2.15	0.79
5:E6:39:ARG:NH2	13:P6:24:TYR:OH	2.16	0.79
1:A6:718:GLN:NE2	5:E6:15:TYR:OH	2.14	0.79
14:A6:1602:CLA:HBB1	14:A6:1651:CLA:HED1	1.64	0.79
8:J5:27:ILE:CG2	16:J5:104:BCR:H343	2.13	0.79
1:A1:270:PHE:CE1	14:A1:840:CLA:HMD2	2.16	0.79
1:A2:578:CYS:SG	18:A2:1655:SF4:FE3	1.73	0.79
14:A4:801:CLA:HBB1	14:B4:804:CLA:HED1	1.65	0.79
2:B4:313:LYS:O	2:B4:314:VAL:HG22	1.83	0.79
2:B5:591:ASN:HB2	14:B5:1804:CLA:HBC2	1.64	0.79
2:B6:509:SER:O	2:B6:511:THR:N	2.12	0.79
2:B6:537:THR:HG21	14:B6:825:CLA:CBB	2.13	0.79
3:C2:57:CYS:SG	18:C2:102:SF4:FE1	1.75	0.79
17:B2:849:LHG:HC2	12:X2:12:ARG:HH21	1.46	0.79
2:B4:434:PHE:CE2	14:B4:802:CLA:C2	2.65	0.79
2:B5:278:ALA:HB2	14:B5:1819:CLA:HBB1	1.64	0.79
14:A2:1644:CLA:H192	10:L2:58:LEU:HD21	1.65	0.79
2:B2:278:ALA:HB2	14:B2:816:CLA:HBB1	1.65	0.79
2:B1:296:ILE:CG1	14:B1:822:CLA:OBD	2.31	0.79
2:B1:727:TYR:HB2	14:B1:804:CLA:HED3	1.64	0.78
2:B1:361:TYR:OH	14:B1:829:CLA:OBD	1.99	0.78
1:A4:423:ALA:HA	4:D4:38:VAL:HG11	1.65	0.78
2:B6:116:TYR:HA	2:B6:370:THR:HG22	1.65	0.78
1:A4:453:PHE:O	14:L4:201:CLA:HBB2	1.83	0.78
1:A2:627:PRO:HB3	1:A5:506:ALA:O	1.84	0.78
4:D4:101:PHE:HB3	4:D4:103:GLU:OE2	1.83	0.78
2:B1:229:TRP:CH2	14:B1:817:CLA:H71	2.17	0.78
1:A3:100:TYR:HA	1:A3:144:PHE:CE1	2.18	0.78
1:A4:207:LEU:HD22	16:A4:845:BCR:H361	1.63	0.78
2:B6:278:ALA:CB	14:B6:817:CLA:HBB1	2.13	0.78
2:B4:566:ASP:OD2	3:C4:65:ARG:NH2	2.16	0.78
14:A3:801:CLA:HBB1	14:B3:1804:CLA:HED1	1.64	0.78
3:C3:50:CYS:SG	18:C3:101:SF4:FE1	1.75	0.78
5:E2:57:THR:HG23	13:P2:42:ALA:HB2	1.65	0.78
10:L1:61:PRO:HB3	14:L1:207:CLA:HBB1	1.65	0.78
1:A6:203:GLY:HA2	14:A6:1620:CLA:HBC1	1.65	0.78
14:L1:205:CLA:HBA2	16:L1:209:BCR:H363	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:180:GLY:HA3	14:B3:1815:CLA:CBB	2.14	0.77
2:B3:493:PRO:HG3	14:B3:1838:CLA:C1D	2.14	0.77
1:A1:203:GLY:HA2	14:A1:819:CLA:HBC1	1.66	0.77
1:A5:203:GLY:HA2	14:A5:820:CLA:HBC1	1.67	0.77
2:B2:430:LEU:HB3	14:B2:831:CLA:HED3	1.66	0.77
3:C6:15:GLN:OE1	13:P6:64:PHE:CE2	2.38	0.77
10:L5:61:PRO:HB3	14:L5:206:CLA:HBB1	1.65	0.77
2:B6:52:HIS:CD2	14:B6:806:CLA:HMA1	2.19	0.77
3:C2:50:CYS:SG	18:C2:101:SF4:FE1	1.75	0.77
1:A1:40:ARG:HD3	13:P1:61:ASP:CA	2.13	0.77
1:A6:464:THR:HG22	1:A6:468:PHE:CE1	2.20	0.77
14:B6:809:CLA:H201	7:I6:23:PRO:HB3	1.67	0.76
1:A5:453:PHE:O	14:L5:203:CLA:HBB2	1.85	0.76
10:L3:33:ASN:O	10:L3:38:ARG:NE	2.18	0.76
1:A3:270:PHE:CD1	14:A3:844:CLA:HMD2	2.20	0.76
11:M4:24:ARG:HH21	14:A6:1601:CLA:HED2	1.49	0.76
1:A6:482:LEU:HB2	1:A6:533:THR:HG23	1.67	0.76
2:B1:59:TRP:CD1	14:B1:808:CLA:HBC1	2.20	0.76
2:B1:65:PHE:CE2	14:B1:809:CLA:C4C	2.68	0.76
2:B3:360:PRO:HG3	14:B3:1820:CLA:HBA1	1.67	0.76
2:B5:622:LEU:HD13	14:B5:1804:CLA:CMA	2.15	0.76
6:F4:65:ILE:CD1	14:J4:102:CLA:HMB3	2.15	0.76
2:B3:166:TRP:CZ2	14:B3:1813:CLA:CMA	2.66	0.76
10:L6:58:LEU:CD2	14:L6:203:CLA:H192	2.15	0.76
2:B6:181:LEU:CD1	14:B6:813:CLA:H43	2.16	0.76
2:B2:354:HIS:ND1	14:B2:816:CLA:OBD	2.16	0.76
11:M6:24:ARG:NH2	14:L5:202:CLA:HED2	2.01	0.76
5:E4:39:ARG:NH1	13:P4:24:TYR:CE2	2.53	0.76
2:B1:466:ILE:HD11	14:B1:838:CLA:O2A	1.84	0.76
1:A1:36:ARG:NH2	13:P1:70:ILE:HG21	2.01	0.76
2:B6:188:ALA:HA	14:B6:815:CLA:CBB	2.16	0.76
2:B1:60:VAL:HG21	14:B1:829:CLA:H11	1.66	0.76
2:B3:300:ILE:HG21	14:B3:1826:CLA:HAC1	1.68	0.76
10:L3:93:LEU:HD21	16:L3:206:BCR:H383	1.66	0.76
1:A6:453:PHE:O	14:A6:1633:CLA:HBB2	1.86	0.75
3:C5:20:CYS:SG	18:C5:101:SF4:FE2	1.79	0.75
6:F6:88:VAL:HG12	6:F6:94:ALA:HA	1.69	0.75
2:B1:339:TRP:CH2	16:B1:846:BCR:H372	2.20	0.75
3:C6:13:CYS:SG	18:C6:102:SF4:FE3	1.79	0.75
8:J1:27:ILE:HG22	16:J1:104:BCR:H343	1.67	0.75
1:A1:336:PHE:HB2	17:A1:849:LHG:HC41	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:453:PHE:O	14:A3:834:CLA:HBB2	1.86	0.75
1:A6:473:ASP:OD2	14:A6:1633:CLA:HED3	1.87	0.75
3:C6:50:CYS:SG	18:C6:101:SF4:FE1	1.79	0.75
6:F2:69:LEU:HB2	14:F2:204:CLA:HBB1	1.69	0.75
1:A1:453:PHE:O	14:L1:202:CLA:HBB2	1.86	0.75
2:B1:60:VAL:HG21	14:B1:829:CLA:H42	1.68	0.75
10:L3:52:MET:HE2	14:L3:203:CLA:H2A	1.67	0.75
11:M2:4:THR:N	11:M2:7:GLN:OE1	2.15	0.75
1:A3:207:LEU:HD22	16:A3:848:BCR:H361	1.67	0.75
2:B6:181:LEU:HD11	14:B6:813:CLA:H43	1.68	0.75
3:C5:13:CYS:SG	18:C5:102:SF4:FE3	1.78	0.75
2:B1:256:PHE:CE1	14:B1:818:CLA:HAB	2.22	0.75
9:K1:73:VAL:CA	14:K1:1401:CLA:HBB1	2.15	0.75
1:A3:352:TRP:CE2	14:A3:825:CLA:H18	2.22	0.74
2:B2:166:TRP:CZ2	14:B2:812:CLA:HAC2	2.21	0.74
14:B2:817:CLA:HBB1	14:B2:817:CLA:HMB1	1.69	0.74
14:B6:818:CLA:HBB1	14:B6:818:CLA:HMB1	1.68	0.74
1:A1:84:PHE:CZ	14:A1:804:CLA:H91	2.22	0.74
1:A1:468:PHE:CZ	14:B1:811:CLA:CHC	2.70	0.74
14:B1:819:CLA:HBB1	14:B1:819:CLA:HMB1	1.70	0.74
2:B3:65:PHE:HE2	14:B3:1809:CLA:CHD	2.00	0.74
2:B5:114:ILE:O	14:B5:1810:CLA:HMD3	1.87	0.74
5:E3:57:THR:HG23	13:P3:42:ALA:HB2	1.68	0.74
2:B2:122:TRP:CZ2	14:B2:812:CLA:H191	2.22	0.74
14:B4:820:CLA:HBB1	14:B4:820:CLA:HMB1	1.69	0.74
2:B4:180:GLY:HA3	14:B4:815:CLA:CBB	2.17	0.74
8:J2:31:ARG:HD3	16:J2:103:BCR:H312	1.69	0.74
1:A3:336:PHE:HB2	17:A3:854:LHG:HC41	1.69	0.74
2:B3:493:PRO:HG3	14:B3:1838:CLA:C4D	2.17	0.74
1:A2:210:LEU:HD21	16:A2:1647:BCR:H342	1.70	0.74
14:B5:1820:CLA:HBB1	14:B5:1820:CLA:HMB1	1.69	0.74
11:M6:24:ARG:HH21	14:L5:202:CLA:HED2	1.51	0.74
2:B3:181:LEU:HD13	14:B3:1815:CLA:HBB	1.69	0.74
14:B3:1820:CLA:HMB1	14:B3:1820:CLA:HBB1	1.70	0.74
3:C1:13:CYS:HG	18:C1:102:SF4:FE3	0.48	0.74
3:C3:11:ILE:CD1	13:P3:39:SER:O	2.36	0.74
10:L4:91:ALA:HA	14:L6:206:CLA:OBD	1.87	0.74
12:X4:26:VAL:HG12	14:X4:102:CLA:HED2	1.69	0.74
4:D1:101:PHE:HB3	4:D1:103:GLU:OE2	1.88	0.74
2:B5:174:LEU:HD21	14:B5:1826:CLA:C1D	2.18	0.74
2:B1:92:ASP:OD2	14:B1:811:CLA:MG	1.31	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:21:TRP:CZ2	14:B3:1842:CLA:CMB	2.67	0.73
2:B4:487:ILE:HG12	14:B4:837:CLA:HMD3	1.70	0.73
14:B4:852:CLA:HBC3	1:A6:333:LYS:O	1.88	0.73
2:B5:339:TRP:HZ2	14:B5:1826:CLA:HAB	1.52	0.73
1:A6:40:ARG:HD3	13:P6:60:SER:O	1.88	0.73
2:B2:278:ALA:CB	14:B2:816:CLA:HBB1	2.18	0.73
3:C5:13:CYS:SG	3:C5:14:THR:O	2.45	0.73
2:B3:48:SER:OG	14:B3:1807:CLA:CBB	2.35	0.73
3:C2:50:CYS:HG	18:C2:101:SF4:FE1	1.02	0.73
6:F4:70:PHE:HE1	16:F4:201:BCR:C10	2.00	0.73
7:I5:30:LEU:O	7:I5:33:TYR:N	2.21	0.73
14:B1:830:CLA:HMB1	14:B1:830:CLA:HBB1	1.69	0.73
2:B6:25:ALA:HB2	19:B6:848:LMG:H121	1.69	0.73
14:B3:1831:CLA:HMB1	14:B3:1831:CLA:HBB1	1.68	0.73
1:A5:281:PHE:HE1	14:A5:818:CLA:HAB	1.50	0.73
2:B4:300:ILE:HG21	14:B4:826:CLA:HAC1	1.71	0.73
2:B5:229:TRP:HB2	14:B5:1818:CLA:H12	1.71	0.73
14:B5:1831:CLA:HBB1	14:B5:1831:CLA:HMB1	1.68	0.73
14:B6:829:CLA:HMB1	14:B6:829:CLA:HBB1	1.69	0.73
3:C4:20:CYS:SG	18:C4:101:SF4:FE2	1.78	0.73
10:L1:86:ILE:O	10:L1:90:THR:OG1	2.07	0.73
1:A3:578:CYS:HB3	1:A3:587:CYS:HA	1.70	0.73
1:A5:677:LEU:HD11	2:B5:623:MET:HB2	1.71	0.73
2:B2:386:MET:HE1	16:B2:846:BCR:H361	1.70	0.73
1:A3:380:TYR:OH	14:A3:829:CLA:OBD	2.07	0.73
1:A6:544:PHE:HZ	14:B6:802:CLA:CBB	2.02	0.73
2:B1:654:TRP:CH2	14:B1:801:CLA:H72	2.23	0.73
3:C5:50:CYS:SG	18:C5:101:SF4:FE1	1.81	0.73
5:E6:37:ILE:CD1	13:P6:41:ARG:CD	2.67	0.73
1:A1:36:ARG:CZ	13:P1:70:ILE:CB	2.67	0.73
1:A2:578:CYS:HB3	1:A2:587:CYS:HA	1.70	0.72
2:B6:321:PRO:HB2	2:B6:409:ASN:HA	1.71	0.72
6:F6:76:TRP:CZ3	14:F6:202:CLA:HBA2	2.24	0.72
1:A2:453:PHE:O	14:L2:202:CLA:HBB2	1.89	0.72
2:B2:622:LEU:HD12	14:B2:802:CLA:H11	1.71	0.72
18:A5:854:SF4:FE4	2:B5:565:CYS:SG	1.81	0.72
6:F6:76:TRP:CE2	14:F6:202:CLA:HBD	2.24	0.72
16:A2:1652:BCR:H321	16:A2:1652:BCR:HC8	1.71	0.72
16:A3:852:BCR:H321	16:A3:852:BCR:HC8	1.71	0.72
2:B1:229:TRP:CB	14:B1:817:CLA:H12	2.19	0.72
11:M4:9:TYR:HB3	16:M4:101:BCR:H401	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:150:PHE:HD2	14:B2:810:CLA:CBC	2.01	0.72
10:L4:56:TYR:OH	14:B5:1812:CLA:H162	1.90	0.72
10:L4:134:VAL:HG23	16:L4:208:BCR:C40	2.17	0.72
12:X4:26:VAL:CB	14:X4:102:CLA:HED1	2.19	0.72
1:A1:36:ARG:NH1	13:P1:70:ILE:CB	2.52	0.72
2:B2:150:PHE:CD2	14:B2:810:CLA:CBC	2.73	0.72
1:A3:333:LYS:O	14:A3:845:CLA:HBC3	1.89	0.72
14:B1:826:CLA:HAA2	14:B1:827:CLA:OBD	1.90	0.72
2:B3:481:LEU:HD11	14:B3:1836:CLA:OBD	1.89	0.72
10:L1:91:ALA:HA	14:L2:205:CLA:OBD	1.89	0.72
2:B2:52:HIS:CE1	14:B2:804:CLA:CMA	2.73	0.72
14:B4:812:CLA:H91	14:L6:208:CLA:C9	2.19	0.72
1:A4:40:ARG:HG2	13:P4:60:SER:O	1.86	0.72
16:A4:849:BCR:HC8	16:A4:849:BCR:H321	1.71	0.71
16:A6:1648:BCR:H321	16:A6:1648:BCR:HC8	1.72	0.71
1:A6:336:PHE:HB2	17:A6:1650:LHG:HC41	1.72	0.71
2:B1:208:TRP:N	14:B1:815:CLA:HMD1	2.04	0.71
3:C5:57:CYS:SG	18:C5:102:SF4:FE1	1.79	0.71
1:A4:202:ALA:HB2	1:A4:312:GLY:HA3	1.72	0.71
2:B2:60:VAL:HG21	14:B2:827:CLA:H11	1.71	0.71
14:B3:1827:CLA:HAA2	14:B3:1828:CLA:OBD	1.90	0.71
14:A2:1604:CLA:C2	2:B2:434:PHE:CE2	2.74	0.71
16:A5:850:BCR:HC8	16:A5:850:BCR:H321	1.72	0.71
1:A5:651:ARG:HB2	2:B5:638:ILE:HG23	1.70	0.71
2:B6:459:GLU:HG3	6:F6:5:LEU:HD11	1.71	0.71
1:A1:202:ALA:HB2	1:A1:312:GLY:HA3	1.71	0.71
1:A5:336:PHE:HB2	17:A5:852:LHG:HC41	1.71	0.71
2:B1:275:HIS:HE2	14:B1:819:CLA:C2B	2.02	0.71
14:B2:824:CLA:HAA2	14:B2:825:CLA:OBD	1.90	0.71
14:B4:831:CLA:HMB1	14:B4:831:CLA:HBB1	1.70	0.71
8:J2:12:PRO:HB2	16:J2:103:BCR:H391	1.72	0.71
1:A2:40:ARG:HD3	13:P2:61:ASP:CA	2.20	0.71
1:A2:203:GLY:HA2	14:A2:1622:CLA:HBC1	1.72	0.71
1:A3:40:ARG:CG	13:P3:60:SER:O	2.37	0.71
2:B3:65:PHE:CE2	14:B3:1809:CLA:C4C	2.72	0.71
2:B4:321:PRO:HB2	2:B4:409:ASN:HA	1.72	0.71
5:E2:57:THR:HG21	13:P2:41:ARG:O	1.90	0.71
10:L4:62:TRP:CZ2	14:L4:201:CLA:C1	2.74	0.71
5:E3:37:ILE:HD13	13:P3:41:ARG:HD2	1.73	0.71
14:B2:828:CLA:HMB1	14:B2:828:CLA:HBB1	1.71	0.71
2:B4:481:LEU:HA	2:B4:489:SER:OG	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A6:578:CYS:SG	18:B6:801:SF4:FE3	1.83	0.71
1:A2:202:ALA:HB2	1:A2:312:GLY:HA3	1.73	0.71
1:A5:202:ALA:HB2	1:A5:312:GLY:HA3	1.71	0.71
6:F6:76:TRP:NE1	14:F6:202:CLA:CBD	2.52	0.71
8:J4:28:GLU:OE2	14:J4:101:CLA:NA	2.24	0.71
1:A5:90:MET:HE2	14:A5:828:CLA:HED1	1.72	0.71
2:B1:430:LEU:HD11	16:B1:848:BCR:C40	2.20	0.71
14:B5:1827:CLA:HAA2	14:B5:1828:CLA:OBD	1.91	0.71
14:B1:811:CLA:H203	7:I1:26:VAL:HG23	1.73	0.71
1:A2:40:ARG:HD3	13:P2:61:ASP:HA	1.72	0.70
14:B1:854:CLA:H91	14:L2:207:CLA:C9	2.18	0.70
2:B2:339:TRP:CZ2	14:B2:823:CLA:HAB	2.24	0.70
14:B4:827:CLA:HAA2	14:B4:828:CLA:OBD	1.91	0.70
14:B6:825:CLA:HAA2	14:B6:826:CLA:OBD	1.90	0.70
3:C3:57:CYS:SG	18:C3:102:SF4:FE1	1.83	0.70
1:A1:352:TRP:HB3	14:A1:804:CLA:HAC1	1.74	0.70
16:A1:847:BCR:H321	16:A1:847:BCR:HC8	1.73	0.70
1:A2:341:HIS:HE1	17:A2:1654:LHG:HC11	1.56	0.70
1:A6:270:PHE:CE1	14:A6:1641:CLA:HMD2	2.27	0.70
2:B2:188:ALA:HA	14:B2:814:CLA:CBB	2.21	0.70
2:B4:521:GLY:HA3	2:B4:619:SER:OG	1.91	0.70
2:B4:425:LEU:HG	14:B4:841:CLA:HBB1	1.72	0.70
2:B5:256:PHE:CE1	14:B5:1819:CLA:HAB	2.27	0.70
2:B6:381:ILE:HD12	14:B6:828:CLA:HBB1	1.71	0.70
3:C2:20:CYS:HG	18:C2:101:SF4:FE2	0.40	0.70
14:B2:808:CLA:H192	7:I2:26:VAL:HG21	1.73	0.70
2:B6:574:CYS:SG	18:B6:801:SF4:FE1	1.82	0.70
3:C5:10:CYS:SG	18:C5:102:SF4:FE4	1.78	0.70
10:L6:124:PHE:CZ	16:L6:209:BCR:H292	2.27	0.70
1:A3:202:ALA:HB2	1:A3:312:GLY:HA3	1.72	0.70
3:C4:50:CYS:SG	18:C4:101:SF4:FE1	1.83	0.70
2:B2:438:GLY:CA	14:B2:832:CLA:HBB1	2.20	0.70
2:B4:281:VAL:HG13	16:B4:845:BCR:C35	2.21	0.70
8:J1:24:GLY:HA3	14:J1:101:CLA:CBB	2.20	0.70
10:L2:94:ALA:O	10:L2:98:LEU:HG	1.92	0.70
1:A2:90:MET:HE1	14:A2:1610:CLA:HAA2	1.72	0.70
1:A3:433:VAL:HA	1:A3:436:HIS:CE1	2.26	0.70
1:A6:86:TRP:HE1	14:A6:1608:CLA:HBA1	1.56	0.70
5:E6:37:ILE:HD13	13:P6:41:ARG:CD	2.17	0.70
14:L4:205:CLA:H13	7:I5:20:TRP:HE3	1.56	0.70
2:B2:52:HIS:CE1	14:B2:804:CLA:HMA1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:430:LEU:CD1	14:B3:1802:CLA:HED3	2.20	0.70
5:E4:39:ARG:NH2	13:P4:24:TYR:OH	2.23	0.70
2:B3:412:ASP:O	2:B3:416:GLN:HG2	1.92	0.70
2:B6:267:LEU:HD22	14:B6:817:CLA:HBA1	1.72	0.70
3:C2:11:ILE:HD11	13:P2:40:CYS:HA	1.73	0.70
1:A1:697:TRP:CH2	15:A1:841:PQN:H2M3	2.26	0.69
1:A5:40:ARG:HG2	13:P5:60:SER:HG	1.51	0.69
1:A6:202:ALA:HB2	1:A6:312:GLY:HA3	1.72	0.69
1:A1:468:PHE:HZ	14:B1:811:CLA:CHC	2.05	0.69
2:B6:243:PHE:H	2:B6:263:GLN:HE22	1.39	0.69
14:A1:801:CLA:HAB	14:B1:804:CLA:C1A	2.21	0.69
2:B1:232:TYR:HB2	14:B1:817:CLA:HMA1	1.73	0.69
2:B1:278:ALA:CB	14:B1:818:CLA:HBB1	2.22	0.69
2:B1:173:ARG:HB3	14:B1:825:CLA:CMD	2.22	0.69
2:B1:349:SER:HB3	14:B1:826:CLA:CAD	2.22	0.69
2:B2:339:TRP:HE1	14:B2:823:CLA:C3B	2.05	0.69
6:F4:65:ILE:HD13	14:J4:102:CLA:HMB3	1.72	0.69
5:E2:3:ARG:CZ	13:P2:31:GLU:HB2	2.21	0.69
1:A3:399:TRP:CD1	14:A3:828:CLA:HAB	2.27	0.69
2:B3:698:ARG:H	10:L3:96:TYR:HH	1.40	0.69
2:B4:434:PHE:CE2	14:B4:802:CLA:H2	2.27	0.69
4:D3:60:ARG:NH2	4:D3:62:GLU:OE2	2.24	0.69
1:A1:468:PHE:CZ	14:B1:811:CLA:C1C	2.76	0.69
1:A2:40:ARG:CZ	13:P2:62:GLN:O	2.40	0.69
12:X2:23:ASN:OD1	14:X2:1701:CLA:C4A	2.40	0.69
1:A4:431:ASP:O	1:A4:435:ARG:HG3	1.92	0.69
2:B2:334:HIS:CE1	2:B2:395:ILE:HG21	2.28	0.69
1:A1:71:LYS:NZ	14:A1:810:CLA:HED2	2.07	0.69
1:A3:94:GLY:O	1:A3:98:SER:OG	2.09	0.69
2:B1:588:TRP:HH2	14:B1:805:CLA:CBB	2.05	0.69
14:A2:1602:CLA:HAB	14:B2:801:CLA:C1A	2.23	0.69
2:B5:466:ILE:HD11	14:B5:1839:CLA:O2A	1.91	0.69
2:B6:60:VAL:HG22	14:B6:828:CLA:H11	1.74	0.69
1:A2:90:MET:HE3	14:A2:1610:CLA:HED2	1.75	0.69
2:B1:539:ILE:HG12	14:B1:802:CLA:HMD1	1.74	0.69
2:B3:229:TRP:HB2	14:B3:1818:CLA:H12	1.74	0.69
10:L4:49:GLU:OE2	14:L4:203:CLA:MG	1.35	0.69
1:A6:40:ARG:CD	13:P6:60:SER:O	2.39	0.69
1:A3:438:ASP:OD1	1:A3:438:ASP:N	2.25	0.69
1:A1:333:LYS:O	14:B3:1801:CLA:HBC3	1.93	0.69
14:A2:1601:CLA:HMD2	10:L2:21:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A4:836:CLA:H101	14:L4:204:CLA:H191	1.74	0.69
2:B4:166:TRP:CZ2	14:B4:813:CLA:HMA1	2.28	0.69
3:C4:50:CYS:HG	18:C4:101:SF4:FE1	1.08	0.69
3:C4:13:CYS:HG	18:C4:102:SF4:FE3	0.46	0.69
1:A4:92:PHE:CZ	14:A4:806:CLA:HMD3	2.27	0.69
1:A5:49:TRP:CZ2	14:A5:840:CLA:HMB1	2.26	0.69
2:B1:275:HIS:HB2	14:B1:818:CLA:C1B	2.22	0.69
2:B2:727:TYR:HB2	14:B2:801:CLA:HED3	1.75	0.69
2:B2:318:PHE:CD1	14:B2:821:CLA:HAB	2.27	0.69
1:A6:587:CYS:SG	18:B6:801:SF4:S4	2.89	0.69
6:F6:76:TRP:CZ2	14:F6:202:CLA:O1A	2.45	0.69
10:L1:134:VAL:HB	16:L1:209:BCR:H403	1.75	0.69
1:A2:36:ARG:NH1	13:P2:71:GLU:HG3	2.08	0.69
1:A4:336:PHE:HB2	17:A4:851:LHG:HC41	1.73	0.69
5:E4:37:ILE:CD1	13:P4:41:ARG:CD	2.70	0.69
1:A3:177:TRP:HB2	14:A3:811:CLA:HMC3	1.75	0.68
14:B4:812:CLA:H203	14:L6:208:CLA:HMD1	1.75	0.68
1:A4:86:TRP:HA	14:A4:806:CLA:HBB2	1.76	0.68
2:B5:278:ALA:CB	14:B5:1819:CLA:HBB1	2.23	0.68
2:B2:60:VAL:HG22	14:B2:827:CLA:H11	1.75	0.68
2:B6:361:TYR:HE2	14:B6:818:CLA:O2D	1.75	0.68
1:A1:177:TRP:HB2	14:A1:810:CLA:HMC3	1.76	0.68
14:A6:1602:CLA:HAB	14:B6:804:CLA:C1A	2.23	0.68
14:A2:1644:CLA:HMA1	2:B2:694:ALA:CB	2.23	0.68
3:C6:20:CYS:SG	18:C6:101:SF4:FE2	1.84	0.68
2:B1:60:VAL:HG22	14:B1:829:CLA:H11	1.74	0.68
2:B1:588:TRP:CH2	14:B1:805:CLA:CBB	2.77	0.68
2:B2:187:LEU:HD11	16:B2:842:BCR:H342	1.75	0.68
10:L5:46:ARG:O	10:L5:50:VAL:HG23	1.94	0.68
1:A4:180:TYR:OH	14:A4:810:CLA:O1D	2.09	0.68
2:B1:28:HIS:HB2	14:B1:830:CLA:CGA	2.23	0.68
2:B1:52:HIS:NE2	14:B1:807:CLA:HMA1	2.08	0.68
2:B4:360:PRO:HG3	14:B4:820:CLA:HBA1	1.76	0.68
2:B5:122:TRP:CZ2	14:B5:1815:CLA:H191	2.29	0.68
2:B5:622:LEU:HD13	14:B5:1804:CLA:HMA2	1.75	0.68
2:B6:654:TRP:NE1	14:B6:802:CLA:H41	2.08	0.68
11:M3:21:LEU:HD21	14:M3:1601:CLA:CMA	2.24	0.68
1:A5:79:HIS:CD2	14:A5:805:CLA:HMA1	2.29	0.68
10:L3:139:LEU:HD23	14:L3:205:CLA:H11	1.75	0.68
1:A2:180:TYR:CE2	14:A2:1613:CLA:C3D	2.77	0.68
1:A3:231:VAL:O	1:A3:232:ALA:HB3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:651:ARG:NE	1:A4:652:ASP:OD2	2.27	0.68
2:B1:116:TYR:HA	2:B1:370:THR:HG22	1.76	0.68
2:B2:25:ALA:HB2	19:B2:848:LMG:H121	1.74	0.68
2:B4:664:ALA:C	14:B4:805:CLA:HBB1	2.15	0.68
2:B6:113:ASP:N	2:B6:113:ASP:OD2	2.27	0.68
2:B6:630:LEU:HD11	14:B6:804:CLA:H93	1.75	0.68
3:C6:16:CYS:SG	3:C6:17:VAL:N	2.67	0.68
6:F4:88:VAL:HG11	6:F4:97:LYS:HB2	1.75	0.68
14:A3:838:CLA:H101	14:L3:204:CLA:H191	1.73	0.68
14:A6:1637:CLA:H101	14:L6:207:CLA:H191	1.76	0.68
2:B3:304:MET:HG3	2:B3:322:HIS:O	1.93	0.68
2:B3:430:LEU:HD13	14:B3:1802:CLA:CED	2.24	0.68
2:B5:433:GLY:HA3	14:B5:1802:CLA:O1A	1.94	0.68
3:C5:20:CYS:SG	3:C5:22:THR:OG1	2.52	0.68
8:J4:27:ILE:HD13	16:J4:104:BCR:C11	2.24	0.68
1:A1:40:ARG:CG	13:P1:61:ASP:HA	2.23	0.68
1:A5:36:ARG:NH1	13:P5:70:ILE:CB	2.56	0.68
1:A3:313:HIS:CE1	16:A3:847:BCR:H363	2.30	0.67
1:A6:231:VAL:O	1:A6:232:ALA:HB3	1.94	0.67
2:B1:28:HIS:HB2	14:B1:830:CLA:HBA1	1.76	0.67
2:B2:521:GLY:HA3	2:B2:619:SER:OG	1.94	0.67
2:B3:591:ASN:HB2	14:B3:1804:CLA:HBC2	1.74	0.67
2:B3:321:PRO:HB2	2:B3:409:ASN:HA	1.76	0.67
2:B6:694:ALA:CB	14:L6:203:CLA:HMA1	2.24	0.67
5:E3:57:THR:HG21	13:P3:41:ARG:O	1.93	0.67
12:X4:26:VAL:HB	14:X4:102:CLA:CED	2.23	0.67
1:A1:86:TRP:HA	14:A1:806:CLA:HBB2	1.76	0.67
14:A4:853:CLA:HAA2	14:B5:1801:CLA:HBA1	1.76	0.67
2:B1:271:ASP:C	14:B1:818:CLA:HMA1	2.14	0.67
2:B3:724:ILE:HD13	19:B3:1850:LMG:C43	2.24	0.67
9:K4:73:VAL:HA	14:K4:1401:CLA:CBB	2.25	0.67
1:A1:726:GLN:HG3	17:A1:848:LHG:O9	1.94	0.67
1:A6:445:ASN:ND2	14:B6:805:CLA:HED2	2.09	0.67
2:B1:442:HIS:HB2	14:B1:834:CLA:C1C	2.24	0.67
2:B3:300:ILE:HD13	14:B3:1826:CLA:CAC	2.25	0.67
14:B4:839:CLA:H51	12:X4:26:VAL:HG11	1.75	0.67
1:A1:231:VAL:O	1:A1:232:ALA:HB3	1.95	0.67
18:A2:1655:SF4:FE1	2:B2:574:CYS:SG	1.82	0.67
1:A4:333:LYS:O	14:B5:1801:CLA:HBC3	1.95	0.67
2:B1:275:HIS:HB2	14:B1:818:CLA:CHB	2.24	0.67
2:B1:525:VAL:CG1	14:B1:804:CLA:H141	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:64:LEU:HD11	16:B2:844:BCR:H271	1.75	0.67
2:B1:53:LEU:HD12	14:B1:807:CLA:O1A	1.94	0.67
2:B1:711:ALA:HB2	15:B1:842:PQN:C8	2.24	0.67
2:B4:192:HIS:HE1	14:B4:816:CLA:C1A	2.08	0.67
5:E6:39:ARG:NH1	13:P6:24:TYR:OH	2.27	0.67
14:L4:203:CLA:CBA	16:L4:208:BCR:H363	2.24	0.67
10:L5:53:ALA:HB2	14:L5:205:CLA:HED3	1.77	0.67
14:A3:801:CLA:HAB	14:B3:1803:CLA:C1A	2.24	0.67
14:A5:801:CLA:HAB	14:B5:1803:CLA:C1A	2.24	0.67
2:B1:230:GLY:N	14:B1:817:CLA:HBA2	2.06	0.67
2:B3:220:GLY:HA3	14:B3:1817:CLA:HMD1	1.77	0.67
2:B4:192:HIS:CE1	14:B4:816:CLA:C4A	2.78	0.67
1:A3:345:TYR:O	1:A3:349:THR:HB	1.94	0.67
1:A3:86:TRP:HA	14:A3:807:CLA:HBB2	1.77	0.67
1:A5:578:CYS:HB3	1:A5:587:CYS:HA	1.75	0.67
17:B2:849:LHG:HC2	12:X2:12:ARG:NH2	2.09	0.67
1:A3:587:CYS:SG	18:A3:855:SF4:S1	2.93	0.67
1:A5:333:LYS:O	14:A5:843:CLA:HBC3	1.94	0.67
2:B1:711:ALA:CB	15:B1:842:PQN:C8	2.73	0.67
2:B3:281:VAL:HG22	16:B3:1845:BCR:C35	2.25	0.67
2:B5:188:ALA:HA	14:B5:1817:CLA:CBB	2.24	0.67
14:A1:827:CLA:H192	16:J1:103:BCR:H14C	1.77	0.67
1:A5:231:VAL:O	1:A5:232:ALA:HB3	1.94	0.67
2:B3:668:MET:SD	14:B3:1805:CLA:MG	1.77	0.67
2:B6:431:PHE:CZ	16:B6:850:BCR:HC41	2.30	0.67
3:C4:77:GLY:HA2	4:D4:60:ARG:NH2	2.09	0.67
16:I1:103:BCR:H292	10:L1:124:PHE:CZ	2.30	0.67
1:A5:36:ARG:NH1	13:P5:71:GLU:N	2.42	0.67
1:A5:177:TRP:HB2	14:A5:811:CLA:HMC3	1.77	0.67
2:B4:41:LEU:O	2:B4:45:ILE:HG12	1.95	0.67
1:A1:578:CYS:HB3	1:A1:587:CYS:HA	1.77	0.66
1:A1:694:ARG:N	2:B1:574:CYS:SG	2.68	0.66
14:B1:853:CLA:HBC3	1:A2:333:LYS:O	1.93	0.66
1:A5:40:ARG:HG3	13:P5:60:SER:HB2	0.67	0.66
2:B1:181:LEU:HD11	14:B1:814:CLA:H12	1.77	0.66
14:A2:1602:CLA:HBB1	14:B2:802:CLA:CED	2.25	0.66
1:A3:456:PHE:HE2	14:B3:1805:CLA:H92	1.60	0.66
14:B3:1843:CLA:H171	7:I3:24:THR:HG23	1.77	0.66
14:B5:1821:CLA:HAA2	14:B5:1826:CLA:HBB1	1.76	0.66
6:F4:77:ILE:HG12	14:F4:202:CLA:ND	2.09	0.66
5:E3:3:ARG:NH2	13:P3:31:GLU:OE1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:303:ALA:HB2	14:A3:818:CLA:HBB1	1.76	0.66
1:A4:231:VAL:O	1:A4:232:ALA:HB3	1.93	0.66
1:A4:92:PHE:CE2	14:A4:806:CLA:CHD	2.78	0.66
2:B3:466:ILE:HD13	14:B3:1836:CLA:HBB1	1.76	0.66
2:B4:59:TRP:HA	14:B4:809:CLA:HBB2	1.77	0.66
2:B4:122:TRP:HH2	16:B4:847:BCR:H391	1.60	0.66
14:A4:853:CLA:HAA2	14:B5:1801:CLA:CBA	2.25	0.66
14:B6:809:CLA:H201	7:I6:23:PRO:CB	2.25	0.66
10:L3:48:LEU:HD13	14:L3:203:CLA:HED2	1.77	0.66
1:A2:675:LEU:HD11	14:A2:1630:CLA:H143	1.76	0.66
14:A5:801:CLA:HBB1	14:B5:1804:CLA:CED	2.24	0.66
1:A3:456:PHE:CE2	14:B3:1805:CLA:H92	2.31	0.66
14:A4:801:CLA:HBB1	14:B4:804:CLA:CED	2.24	0.66
2:B4:725:LEU:HD11	14:B4:831:CLA:H203	1.77	0.66
6:F2:65:ILE:HD12	14:F2:204:CLA:HMB3	1.75	0.66
6:F6:76:TRP:CD1	14:F6:202:CLA:HBD	2.30	0.66
10:L3:61:PRO:HB3	14:L3:205:CLA:CBB	2.23	0.66
14:A3:802:CLA:H41	2:B3:654:TRP:NE1	2.10	0.66
2:B5:150:PHE:HZ	14:B5:1801:CLA:H2	1.60	0.66
14:B2:806:CLA:H43	7:I2:14:PHE:CE1	2.29	0.66
1:A1:682:ILE:HD11	16:A1:847:BCR:C14	2.26	0.66
18:A1:850:SF4:S3	2:B1:565:CYS:SG	2.93	0.66
2:B3:599:TYR:CD2	14:B3:1839:CLA:HMC2	2.29	0.66
1:A4:445:ASN:ND2	14:B4:805:CLA:HED2	2.10	0.66
2:B4:481:LEU:HD12	14:B4:836:CLA:HED3	1.76	0.66
1:A5:597:LEU:HD13	14:B5:1805:CLA:HMD3	1.78	0.66
14:B3:1801:CLA:CBA	14:M3:1601:CLA:HAA2	2.26	0.66
2:B6:554:PRO:HD2	3:C6:61:PHE:CE1	2.31	0.66
3:C2:10:CYS:SG	18:C2:102:SF4:FE4	1.88	0.66
16:L5:201:BCR:H363	14:L5:204:CLA:HBA2	1.77	0.66
1:A4:592:TRP:CD1	14:A4:829:CLA:HMD1	2.29	0.66
14:A5:828:CLA:H192	16:J5:103:BCR:H14C	1.78	0.66
2:B2:724:ILE:HD13	14:B2:826:CLA:HMC2	1.77	0.66
2:B3:25:ALA:HB2	19:B3:1850:LMG:H121	1.75	0.66
2:B4:182:PHE:CE2	14:B4:815:CLA:H61	2.31	0.66
14:A4:801:CLA:HAB	14:B4:803:CLA:C1A	2.25	0.66
2:B5:52:HIS:CE1	14:B5:1807:CLA:HMA1	2.29	0.66
10:L3:138:LEU:HD13	14:L3:205:CLA:C9	2.25	0.66
1:A3:180:TYR:CE2	14:A3:811:CLA:C3D	2.79	0.66
1:A3:681:PHE:CD2	16:A3:852:BCR:H363	2.31	0.66
1:A5:40:ARG:CG	13:P5:60:SER:OG	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:321:PRO:HB2	2:B1:409:ASN:HA	1.77	0.66
2:B2:339:TRP:HZ2	14:B2:823:CLA:CAB	2.09	0.66
2:B3:122:TRP:CZ2	14:B3:1815:CLA:H191	2.30	0.66
3:C1:10:CYS:SG	18:C1:102:SF4:S3	2.93	0.66
2:B4:221:LEU:HD11	16:B4:845:BCR:HC22	1.78	0.66
14:A2:1639:CLA:H101	14:L2:206:CLA:H191	1.76	0.66
1:A1:79:HIS:CE1	14:A1:804:CLA:HMA2	2.31	0.66
2:B5:664:ALA:HB3	14:B5:1805:CLA:HBB2	1.78	0.66
7:I4:20:TRP:HE1	16:I4:102:BCR:HC22	1.57	0.66
1:A2:651:ARG:NE	1:A2:652:ASP:OD2	2.29	0.65
1:A5:431:ASP:O	1:A5:435:ARG:HG3	1.95	0.65
14:A6:1602:CLA:HBB1	14:A6:1651:CLA:CED	2.25	0.65
2:B1:525:VAL:HG12	14:B1:804:CLA:C14	2.25	0.65
14:B6:837:CLA:HMB2	14:B6:839:CLA:HED1	1.78	0.65
1:A2:423:ALA:HA	4:D2:38:VAL:HG11	1.77	0.65
1:A6:697:TRP:CZ2	15:A6:1642:PQN:H2M3	2.30	0.65
2:B1:298:HIS:HE1	14:B1:823:CLA:OBD	1.74	0.65
2:B1:727:TYR:HB2	14:B1:804:CLA:CED	2.27	0.65
2:B3:498:VAL:HG11	14:B3:1818:CLA:HED2	1.77	0.65
2:B4:318:PHE:HB2	14:B4:825:CLA:HMA1	1.77	0.65
1:A5:597:LEU:HD13	14:B5:1805:CLA:CMD	2.25	0.65
2:B5:493:PRO:HG3	14:B5:1838:CLA:C1D	2.26	0.65
3:C1:20:CYS:HG	18:C1:101:SF4:FE2	0.42	0.65
8:J4:27:ILE:CG2	16:J4:104:BCR:H343	2.26	0.65
2:B6:361:TYR:OH	14:B6:818:CLA:HBD	1.95	0.65
1:A1:592:TRP:CD1	14:A1:829:CLA:HMD1	2.32	0.65
1:A2:231:VAL:O	1:A2:232:ALA:HB3	1.95	0.65
1:A3:249:MET:O	1:A3:252:LEU:O	2.15	0.65
1:A6:439:ALA:HA	2:B6:686:TRP:CZ3	2.31	0.65
2:B1:229:TRP:O	14:B1:817:CLA:H3A	1.96	0.65
2:B2:386:MET:CE	16:B2:846:BCR:H361	2.27	0.65
14:A3:801:CLA:HBB1	14:B3:1804:CLA:CED	2.25	0.65
3:C5:17:VAL:HA	3:C5:25:LEU:HD12	1.78	0.65
6:F1:69:LEU:HB2	14:J1:102:CLA:CBB	2.27	0.65
6:F6:53:VAL:HG12	6:F6:63:PHE:HB2	1.78	0.65
8:J6:12:PRO:HB2	16:J6:1105:BCR:H391	1.78	0.65
16:L6:201:BCR:H363	14:L6:206:CLA:HBA2	1.77	0.65
1:A2:249:MET:O	1:A2:252:LEU:O	2.15	0.65
14:A1:838:CLA:HMC3	14:B1:802:CLA:H71	1.79	0.65
2:B3:360:PRO:HG3	14:B3:1820:CLA:CBA	2.26	0.65
2:B5:116:TYR:HA	2:B5:370:THR:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C3:53:CYS:HG	18:C3:101:SF4:FE3	1.09	0.65
1:A1:36:ARG:CZ	13:P1:70:ILE:HG21	2.26	0.65
1:A4:249:MET:O	1:A4:252:LEU:O	2.15	0.65
1:A6:681:PHE:CD2	16:A6:1648:BCR:H363	2.32	0.65
1:A6:688:MET:SD	14:A6:1603:CLA:MG	1.77	0.65
14:B1:806:CLA:H111	16:B1:849:BCR:H362	1.79	0.65
2:B1:466:ILE:HD11	14:B1:838:CLA:H43	1.77	0.65
2:B2:551:LYS:NZ	6:F2:137:THR:OG1	2.29	0.65
2:B4:181:LEU:HD11	14:B4:815:CLA:H12	1.79	0.65
14:B4:835:CLA:H122	6:F4:69:LEU:HD11	1.79	0.65
10:L2:134:VAL:HG23	16:L2:201:BCR:H403	1.78	0.65
1:A1:36:ARG:CZ	13:P1:70:ILE:HB	2.27	0.65
1:A3:79:HIS:CD2	14:A3:805:CLA:HMA1	2.32	0.65
1:A6:308:PHE:HE2	14:A6:1621:CLA:HAB	1.61	0.65
1:A6:249:MET:O	1:A6:252:LEU:O	2.15	0.65
2:B2:438:GLY:C	14:B2:832:CLA:HBB1	2.17	0.65
8:J4:12:PRO:HB2	16:J4:104:BCR:H391	1.77	0.65
14:B1:820:CLA:HAA2	14:B1:825:CLA:HBB1	1.78	0.65
14:B2:836:CLA:HMB2	14:B2:838:CLA:HED1	1.79	0.65
10:L1:98:LEU:HD21	10:L2:41:LEU:HD21	1.78	0.65
1:A2:399:TRP:CD1	14:A2:1630:CLA:HAB	2.31	0.65
2:B3:192:HIS:HB2	14:B3:1816:CLA:CHC	2.27	0.65
2:B4:377:HIS:HB2	14:B4:829:CLA:C1B	2.26	0.65
3:C3:53:CYS:SG	18:C3:101:SF4:FE3	1.89	0.65
8:J1:27:ILE:HG21	16:J1:104:BCR:C34	2.26	0.65
1:A1:36:ARG:HH12	13:P1:70:ILE:HG12	1.61	0.65
1:A6:177:TRP:HB2	14:A6:1611:CLA:HMC3	1.77	0.65
2:B1:28:HIS:HB2	14:B1:830:CLA:CBA	2.26	0.65
2:B1:274:HIS:HB3	14:B1:818:CLA:CMB	2.26	0.65
14:B3:1821:CLA:HAA2	14:B3:1826:CLA:HBB1	1.77	0.65
2:B5:321:PRO:HB2	2:B5:409:ASN:HA	1.79	0.65
2:B5:79:ASP:O	2:B5:83:THR:OG1	2.13	0.65
2:B6:430:LEU:HB3	14:B6:832:CLA:HED3	1.79	0.65
3:C6:57:CYS:SG	18:C6:102:SF4:FE1	1.89	0.65
12:X3:12:ARG:HB3	17:X3:101:LHG:C5	2.27	0.65
14:A3:828:CLA:H192	16:J3:103:BCR:H14C	1.78	0.64
1:A4:92:PHE:HZ	14:A4:806:CLA:HMD3	1.60	0.64
2:B2:425:LEU:CG	14:B2:838:CLA:CBB	2.69	0.64
2:B3:282:LEU:HD12	14:B3:1821:CLA:HMC1	1.78	0.64
14:A1:839:CLA:H192	10:L1:58:LEU:HD21	1.79	0.64
2:B3:698:ARG:N	10:L3:96:TYR:OH	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:40:ARG:CA	13:P5:60:SER:HB2	2.26	0.64
1:A1:40:ARG:NH1	13:P1:61:ASP:O	2.30	0.64
1:A1:196:MET:HE2	14:A1:812:CLA:HBC2	1.78	0.64
2:B1:279:ILE:CD1	14:B1:818:CLA:CBC	2.75	0.64
14:B5:1825:CLA:HBB1	14:B5:1832:CLA:HMD2	1.79	0.64
2:B6:438:GLY:CA	14:B6:833:CLA:HBB1	2.26	0.64
10:L4:89:ALA:HB1	16:L4:206:BCR:H401	1.78	0.64
1:A4:443:HIS:CD2	14:A4:830:CLA:HMB1	2.32	0.64
1:A5:319:TRP:CD1	14:A5:820:CLA:O1A	2.50	0.64
2:B1:212:LEU:HD21	16:B1:845:BCR:H341	1.78	0.64
2:B3:256:PHE:CD1	14:B3:1819:CLA:HAB	2.32	0.64
2:B4:114:ILE:O	14:B4:810:CLA:HMD3	1.98	0.64
1:A1:210:LEU:HD21	16:A1:842:BCR:H342	1.78	0.64
1:A2:94:GLY:O	1:A2:98:SER:OG	2.14	0.64
14:A4:827:CLA:H192	16:J4:103:BCR:H14C	1.77	0.64
1:A5:249:MET:O	1:A5:252:LEU:O	2.14	0.64
1:A5:360:LEU:CD1	14:A5:830:CLA:HBB1	2.28	0.64
2:B1:479:THR:HG21	12:X1:29:TYR:O	1.98	0.64
2:B2:321:PRO:HB2	2:B2:409:ASN:HA	1.79	0.64
2:B3:114:ILE:O	14:B3:1810:CLA:HMD3	1.97	0.64
16:A3:856:BCR:H362	14:B3:1805:CLA:H111	1.79	0.64
2:B4:487:ILE:HG12	14:B4:837:CLA:CMD	2.27	0.64
2:B6:691:THR:O	2:B6:695:ASN:OD1	2.15	0.64
1:A1:249:MET:O	1:A1:252:LEU:O	2.14	0.64
14:A1:801:CLA:HBB1	14:B1:805:CLA:CED	2.26	0.64
2:B1:229:TRP:HB2	14:B1:817:CLA:CGA	2.27	0.64
2:B1:230:GLY:HA2	14:B1:817:CLA:CAA	2.25	0.64
2:B1:350:LEU:CA	14:B1:826:CLA:HED3	2.27	0.64
2:B4:466:ILE:HD11	14:B4:839:CLA:O2A	1.98	0.64
14:A3:828:CLA:H93	16:J3:103:BCR:H361	1.80	0.64
1:A3:210:LEU:HD21	16:A3:847:BCR:H342	1.79	0.64
18:A5:854:SF4:S3	2:B5:565:CYS:SG	2.93	0.64
14:B3:1839:CLA:HMB2	14:B3:1841:CLA:HED1	1.80	0.64
2:B3:622:LEU:HD12	14:B3:1804:CLA:C1	2.25	0.64
2:B3:693:LEU:HD12	14:L3:204:CLA:H11	1.79	0.64
2:B5:592:THR:O	2:B5:596:VAL:HG13	1.98	0.64
14:B2:806:CLA:CMD	7:I2:10:LEU:HD23	2.28	0.64
1:A2:36:ARG:CZ	13:P2:71:GLU:HG3	2.27	0.64
2:B2:537:THR:HG21	14:B2:824:CLA:CBB	2.28	0.64
2:B3:433:GLY:HA3	14:B3:1802:CLA:O1A	1.97	0.64
14:B4:852:CLA:HMA2	14:A6:1601:CLA:HBD	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:587:CYS:SG	18:A3:855:SF4:FE2	1.88	0.64
1:A6:86:TRP:HA	14:A6:1607:CLA:HBB2	1.80	0.64
14:A6:1633:CLA:HMA2	10:L6:65:LEU:HB3	1.79	0.64
1:A6:345:TYR:O	1:A6:349:THR:HB	1.98	0.64
2:B3:173:ARG:HB2	14:B3:1815:CLA:HBC2	1.79	0.64
1:A3:445:ASN:ND2	14:B3:1805:CLA:HED2	2.13	0.64
14:B6:819:CLA:HAA2	14:B6:824:CLA:HBB1	1.77	0.64
6:F2:88:VAL:HG11	6:F2:97:LYS:HB2	1.80	0.64
8:J5:26:LEU:HD23	16:J5:103:BCR:HC7	1.78	0.64
14:A6:1628:CLA:H192	16:J6:1104:BCR:H14C	1.79	0.64
10:L6:79:LEU:HD22	10:L6:136:PHE:CG	2.32	0.64
1:A4:180:TYR:CE2	14:A4:810:CLA:C3D	2.81	0.64
14:A5:808:CLA:HMC2	14:A5:828:CLA:H142	1.79	0.64
2:B1:275:HIS:CE1	14:B1:818:CLA:C1D	2.80	0.64
2:B3:52:HIS:CE1	14:B3:1807:CLA:HMA1	2.32	0.64
2:B3:446:VAL:HG13	2:B3:451:THR:O	1.98	0.64
16:A5:853:BCR:H362	14:B5:1805:CLA:H111	1.80	0.64
14:A2:1630:CLA:H192	16:J2:102:BCR:H14C	1.79	0.64
10:L6:89:ALA:HB2	14:L6:203:CLA:C14	2.28	0.64
1:A2:281:PHE:HE1	14:A2:1620:CLA:HAB	1.63	0.64
2:B1:350:LEU:N	14:B1:826:CLA:HED3	2.13	0.64
2:B3:339:TRP:HE1	14:B3:1826:CLA:C2B	2.11	0.64
2:B4:664:ALA:HB3	14:B4:805:CLA:HBB2	1.80	0.64
3:C2:47:CYS:SG	18:C2:101:SF4:FE4	1.89	0.64
14:A3:808:CLA:HMC2	14:A3:828:CLA:H142	1.79	0.63
1:A5:313:HIS:NE2	16:A5:845:BCR:H363	2.13	0.63
1:A5:303:ALA:CB	14:A5:818:CLA:HBB1	2.27	0.63
2:B1:339:TRP:CZ3	14:B1:824:CLA:HBC2	2.33	0.63
2:B4:52:HIS:CE1	14:B4:807:CLA:HMA1	2.33	0.63
2:B5:237:ASP:N	2:B5:237:ASP:OD1	2.31	0.63
7:I4:20:TRP:NE1	16:I4:102:BCR:C2	2.56	0.63
14:A1:807:CLA:HMC2	14:A1:827:CLA:H142	1.78	0.63
1:A2:50:ASN:OD1	17:A2:1653:LHG:HC11	1.98	0.63
1:A3:612:HIS:CE1	14:A3:837:CLA:C2C	2.81	0.63
14:A4:807:CLA:HMC2	14:A4:827:CLA:H142	1.80	0.63
2:B2:267:LEU:HD22	14:B2:816:CLA:HBA1	1.79	0.63
2:B5:52:HIS:CE1	14:B5:1807:CLA:CMA	2.81	0.63
2:B6:599:TYR:CZ	14:B6:837:CLA:HBC2	2.33	0.63
1:A6:544:PHE:CZ	14:B6:802:CLA:CBB	2.81	0.63
2:B1:177:HIS:HB3	14:B1:825:CLA:HED3	1.79	0.63
1:A4:399:TRP:CD1	14:A4:827:CLA:HAB	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A6:180:TYR:CE2	14:A6:1611:CLA:C3D	2.82	0.63
2:B3:487:ILE:O	14:B3:1837:CLA:HMD3	1.98	0.63
14:A4:840:CLA:HMC3	14:B4:802:CLA:H71	1.81	0.63
2:B4:188:ALA:HB2	14:B4:830:CLA:H202	1.79	0.63
8:J3:24:GLY:HA3	14:J3:101:CLA:HBB1	1.79	0.63
3:C3:11:ILE:CD1	13:P3:40:CYS:HA	2.28	0.63
14:A5:841:CLA:HMC3	14:B5:1802:CLA:H71	1.80	0.63
15:A5:844:PQN:H172	16:B5:1850:BCR:H382	1.81	0.63
1:A6:681:PHE:CG	16:A6:1648:BCR:H363	2.34	0.63
1:A6:360:LEU:CD1	14:A6:1630:CLA:HBB1	2.28	0.63
14:B1:838:CLA:HMB2	14:B1:840:CLA:HED1	1.78	0.63
2:B2:430:LEU:HB3	14:B2:831:CLA:CED	2.28	0.63
2:B3:176:HIS:ND1	14:B3:1815:CLA:HMC2	2.14	0.63
14:A5:802:CLA:H41	2:B5:654:TRP:CD1	2.33	0.63
1:A2:281:PHE:CE1	14:A2:1620:CLA:HAB	2.34	0.63
1:A6:352:TRP:HE1	14:A6:1625:CLA:H191	1.63	0.63
2:B1:232:TYR:HB2	14:B1:817:CLA:CMA	2.28	0.63
2:B1:527:HIS:CD2	16:B1:852:BCR:HC21	2.34	0.63
14:A2:1604:CLA:O1A	2:B2:531:LEU:HD11	1.99	0.63
10:L6:142:PHE:CE1	14:L6:208:CLA:C1	2.78	0.63
1:A4:578:CYS:HB3	1:A4:587:CYS:HA	1.79	0.63
14:A6:1628:CLA:H93	16:J6:1104:BCR:H361	1.80	0.63
2:B1:275:HIS:HE1	14:B1:818:CLA:CHD	2.12	0.63
2:B3:214:THR:O	14:B3:1817:CLA:HED1	1.99	0.63
14:B4:805:CLA:H111	16:B4:850:BCR:H362	1.79	0.63
14:B4:839:CLA:HMB2	14:B4:841:CLA:HED1	1.80	0.63
1:A3:390:GLN:HE21	1:A3:390:GLN:HA	1.63	0.63
1:A5:84:PHE:CZ	14:A5:805:CLA:H91	2.33	0.63
1:A5:352:TRP:HB3	14:A5:805:CLA:HAC1	1.80	0.63
1:A5:366:LEU:HD11	14:A5:819:CLA:H71	1.81	0.63
14:A5:819:CLA:HMB1	14:A5:819:CLA:HBB1	1.81	0.63
2:B3:42:TYR:OH	2:B3:333:LEU:HD21	1.98	0.63
2:B5:724:ILE:HD13	14:B5:1829:CLA:HMC2	1.81	0.63
14:A1:835:CLA:H101	14:L1:206:CLA:H191	1.80	0.63
10:L3:89:ALA:HB1	16:L3:206:BCR:H401	1.80	0.63
10:L4:61:PRO:HB3	14:L4:205:CLA:HBB1	1.81	0.63
1:A2:86:TRP:HA	14:A2:1609:CLA:HBB2	1.81	0.63
1:A3:90:MET:HE3	14:A3:808:CLA:HED2	1.79	0.63
1:A5:83:VAL:HG11	14:A5:805:CLA:H72	1.80	0.63
2:B3:430:LEU:HD11	16:F3:201:BCR:C40	2.29	0.63
4:D2:60:ARG:NH2	4:D2:62:GLU:OE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A2:1610:CLA:HMC2	14:A2:1630:CLA:H142	1.80	0.62
1:A4:303:ALA:HB2	14:A4:817:CLA:HBB1	1.81	0.62
1:A4:686:SER:HB3	1:A4:734:HIS:HB2	1.81	0.62
2:B1:480:LEU:C	2:B1:482:SER:H	2.03	0.62
2:B6:480:LEU:C	2:B6:482:SER:H	2.02	0.62
1:A6:600:PHE:CD1	14:B6:805:CLA:HBC1	2.34	0.62
5:E3:57:THR:HG21	13:P3:42:ALA:HA	1.81	0.62
8:J5:27:ILE:HG22	16:J5:104:BCR:H343	1.81	0.62
1:A1:19:ASP:HA	1:A1:181:HIS:O	1.99	0.62
1:A4:463:ASP:OD2	2:B4:641:TYR:OH	2.17	0.62
1:A5:688:MET:O	1:A5:692:SER:OG	2.16	0.62
1:A5:86:TRP:HA	14:A5:807:CLA:HBB2	1.80	0.62
2:B3:195:HIS:CE1	14:B3:1816:CLA:HBC1	2.34	0.62
2:B4:531:LEU:HD11	14:B4:802:CLA:O1A	1.99	0.62
2:B5:153:TRP:CH2	14:B5:1801:CLA:C6	2.82	0.62
2:B5:381:ILE:HD12	14:B5:1830:CLA:HBB1	1.81	0.62
3:C5:40:SER:CB	3:C5:41:SER:HA	2.28	0.62
6:F1:88:VAL:HG11	6:F1:97:LYS:HB2	1.81	0.62
6:F5:76:TRP:NE1	14:F5:1301:CLA:HBD	2.13	0.62
8:J5:27:ILE:HG21	16:J5:104:BCR:C9	2.29	0.62
8:J5:31:ARG:HD3	16:J5:104:BCR:C31	2.23	0.62
8:J6:24:GLY:HA3	14:J6:1102:CLA:HBB1	1.80	0.62
9:K2:73:VAL:CA	14:K2:1401:CLA:HBB1	2.08	0.62
10:L2:124:PHE:CE1	16:L2:208:BCR:H292	2.35	0.62
5:E3:57:THR:CG2	13:P3:42:ALA:HA	2.29	0.62
1:A1:79:HIS:ND1	14:A1:804:CLA:O1A	2.30	0.62
2:B1:479:THR:O	2:B1:482:SER:HB3	1.99	0.62
14:A1:801:CLA:HAB	14:B1:804:CLA:NA	2.14	0.62
8:J3:12:PRO:HB2	16:J3:104:BCR:H391	1.81	0.62
10:L6:54:HIS:HA	10:L6:57:PHE:CE2	2.35	0.62
11:M3:13:VAL:HG23	16:M3:1602:BCR:H402	1.81	0.62
1:A2:303:ALA:HB2	14:A2:1620:CLA:HBB1	1.81	0.62
14:B1:854:CLA:H162	10:L2:56:TYR:OH	1.98	0.62
1:A2:686:SER:HB3	1:A2:734:HIS:HB2	1.80	0.62
14:B2:808:CLA:H203	7:I2:26:VAL:HG23	1.81	0.62
6:F2:65:ILE:CD1	14:F2:204:CLA:HMB3	2.29	0.62
7:I4:20:TRP:CE2	16:I4:102:BCR:C3	2.82	0.62
14:A3:819:CLA:HBB1	14:A3:819:CLA:HMB1	1.82	0.62
1:A5:303:ALA:HB2	14:A5:818:CLA:HBB1	1.80	0.62
2:B1:587:PHE:CG	14:B1:802:CLA:HAC2	2.35	0.62
2:B2:503:TRP:HE3	14:B2:816:CLA:H11	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B5:599:TYR:CD2	14:B5:1839:CLA:HMC2	2.34	0.62
2:B5:731:LEU:CD2	14:B5:1829:CLA:CMB	2.77	0.62
2:B6:122:TRP:CH2	14:B6:813:CLA:H201	2.35	0.62
2:B6:60:VAL:CG2	14:B6:828:CLA:H11	2.29	0.62
1:A4:40:ARG:HD3	13:P4:60:SER:O	1.98	0.62
15:A1:841:PQN:H172	16:B1:848:BCR:H382	1.82	0.62
1:A3:352:TRP:HE1	14:A3:825:CLA:H191	1.64	0.62
1:A4:683:TRP:CE2	14:A4:801:CLA:HBA2	2.34	0.62
16:A6:1652:BCR:H362	14:B6:805:CLA:H111	1.80	0.62
2:B3:318:PHE:HB2	14:B3:1825:CLA:HMA1	1.81	0.62
2:B4:480:LEU:C	2:B4:482:SER:H	2.02	0.62
2:B4:2:THR:OG1	2:B4:4:PHE:O	2.18	0.62
2:B4:727:TYR:HB2	14:B4:803:CLA:HED3	1.80	0.62
2:B5:588:TRP:O	2:B5:592:THR:OG1	2.17	0.62
10:L4:62:TRP:CE2	14:L4:201:CLA:C1	2.83	0.62
5:E2:3:ARG:NH1	13:P2:31:GLU:HB2	2.14	0.62
12:X4:23:ASN:HD21	14:X4:102:CLA:C1A	2.13	0.62
1:A4:300:HIS:O	1:A4:304:ILE:HG12	2.00	0.62
2:B2:275:HIS:HB2	14:B2:816:CLA:C1B	2.30	0.62
2:B2:480:LEU:C	2:B2:482:SER:H	2.03	0.62
2:B3:300:ILE:HD13	14:B3:1826:CLA:HAC2	1.82	0.62
2:B6:595:TRP:CD1	14:B6:804:CLA:H152	2.35	0.62
2:B6:52:HIS:CE1	14:B6:806:CLA:CMA	2.83	0.62
1:A1:681:PHE:CG	16:A1:847:BCR:H363	2.35	0.62
18:A3:855:SF4:S3	2:B3:565:CYS:SG	2.98	0.62
2:B5:480:LEU:C	2:B5:482:SER:H	2.03	0.62
15:A3:846:PQN:H172	16:F3:201:BCR:H382	1.82	0.62
3:C4:11:ILE:CD1	13:P4:40:CYS:HA	2.30	0.62
1:A4:19:ASP:HA	1:A4:181:HIS:O	2.00	0.62
15:A4:843:PQN:H172	16:F4:201:BCR:H382	1.81	0.62
14:B4:821:CLA:HAA2	14:B4:826:CLA:HBB1	1.81	0.62
2:B6:275:HIS:HB2	14:B6:817:CLA:C1B	2.30	0.62
12:X3:9:TYR:O	12:X3:10:ALA:HB2	1.99	0.62
14:A1:827:CLA:H93	16:J1:103:BCR:H361	1.82	0.61
2:B1:181:LEU:CD1	14:B1:814:CLA:H43	2.30	0.61
14:B4:842:CLA:HED3	7:I4:31:PHE:HZ	1.65	0.61
16:L3:201:BCR:H363	14:L3:203:CLA:HBA2	1.82	0.61
1:A1:544:PHE:HZ	14:B1:801:CLA:CBB	2.13	0.61
14:A2:1604:CLA:H71	14:A2:1643:CLA:HMC3	1.82	0.61
1:A2:305:ALA:O	1:A2:309:ILE:HG12	2.00	0.61
1:A2:336:PHE:HB2	17:A2:1654:LHG:HC41	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B2:803:CLA:H111	16:B2:847:BCR:H362	1.82	0.61
14:B3:1808:CLA:H102	14:B3:1808:CLA:H151	1.82	0.61
2:B3:529:ILE:HG21	14:B3:1839:CLA:CAB	2.31	0.61
14:A6:1603:CLA:O1A	2:B6:531:LEU:HD11	2.00	0.61
2:B6:592:THR:O	2:B6:596:VAL:HG13	2.00	0.61
1:A4:567:PRO:HD2	4:D4:62:GLU:OE1	2.01	0.61
6:F4:70:PHE:CE1	16:F4:201:BCR:C9	2.83	0.61
14:A1:818:CLA:HMB1	14:A1:818:CLA:HBB1	1.82	0.61
15:A2:1646:PQN:H172	16:F2:201:BCR:H382	1.81	0.61
1:A5:744:TRP:CZ2	14:A5:828:CLA:H11	2.35	0.61
1:A6:431:ASP:O	1:A6:435:ARG:HG3	1.99	0.61
14:B1:824:CLA:HBB1	14:B1:831:CLA:HMD2	1.82	0.61
14:A3:842:CLA:HMC3	14:B3:1802:CLA:H71	1.82	0.61
2:B6:60:VAL:HG21	14:B6:828:CLA:H42	1.81	0.61
2:B6:595:TRP:NE1	14:B6:804:CLA:H152	2.14	0.61
7:I4:36:GLY:HA2	10:L4:102:GLN:HE22	1.65	0.61
14:A4:841:CLA:H192	10:L4:58:LEU:HD21	1.82	0.61
11:M4:29:LEU:O	11:M4:30:TYR:HB2	1.99	0.61
12:X4:26:VAL:CB	14:X4:102:CLA:CED	2.78	0.61
1:A1:399:TRP:CD1	14:A1:827:CLA:HAB	2.35	0.61
1:A2:303:ALA:CB	14:A2:1620:CLA:HBB1	2.30	0.61
1:A2:36:ARG:NH1	13:P2:67:ASP:C	2.52	0.61
15:A6:1642:PQN:H172	16:F6:201:BCR:H382	1.82	0.61
2:B3:340:HIS:HD2	14:B3:1807:CLA:OBD	1.83	0.61
2:B3:529:ILE:HG21	14:B3:1839:CLA:HAB	1.81	0.61
1:A6:650:LEU:HD22	2:B6:657:LEU:HD21	1.83	0.61
8:J1:27:ILE:HG21	16:J1:104:BCR:C9	2.29	0.61
1:A3:681:PHE:CG	16:A3:852:BCR:H363	2.34	0.61
1:A5:28:TRP:CZ2	14:A5:804:CLA:H11	2.36	0.61
2:B1:279:ILE:HD11	14:B1:818:CLA:C3C	2.31	0.61
2:B2:456:ILE:HG22	2:B2:458:ILE:HD11	1.82	0.61
6:F6:76:TRP:CZ2	14:F6:202:CLA:O2D	2.53	0.61
1:A1:40:ARG:HD3	13:P1:61:ASP:CB	2.31	0.61
1:A4:303:ALA:CB	14:A4:817:CLA:HBB1	2.30	0.61
1:A4:429:VAL:O	1:A4:433:VAL:HG13	2.01	0.61
14:A6:1608:CLA:HMC2	14:A6:1628:CLA:H142	1.81	0.61
2:B1:181:LEU:HD21	14:B1:807:CLA:H93	1.83	0.61
2:B1:271:ASP:HB3	14:B1:818:CLA:HMA1	1.81	0.61
14:B4:825:CLA:HBB1	14:B4:832:CLA:HMD2	1.83	0.61
3:C4:30:TRP:O	3:C4:36:GLY:HA2	2.01	0.61
4:D3:50:ARG:H	4:D3:54:ASN:HD21	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D3:60:ARG:N	4:D3:63:GLN:OE1	2.30	0.61
10:L5:33:ASN:O	10:L5:38:ARG:NE	2.29	0.61
10:L5:97:GLY:HA3	10:L5:117:TRP:CD1	2.35	0.61
14:A2:1621:CLA:HBB1	14:A2:1621:CLA:HMB1	1.81	0.61
1:A3:682:ILE:HD11	16:A3:852:BCR:C14	2.30	0.61
1:A4:681:PHE:CD2	16:A4:849:BCR:H363	2.35	0.61
1:A6:473:ASP:HA	10:L6:69:ARG:HH22	1.66	0.61
2:B2:654:TRP:CE2	14:B2:808:CLA:HMC2	2.35	0.61
2:B4:668:MET:SD	14:B4:805:CLA:ND	2.73	0.61
3:C3:30:TRP:O	3:C3:36:GLY:HA2	2.01	0.61
3:C6:30:TRP:O	3:C6:36:GLY:HA2	2.00	0.61
5:E3:57:THR:HG23	13:P3:42:ALA:CB	2.30	0.61
14:A2:1630:CLA:H93	16:J2:102:BCR:H361	1.81	0.61
1:A3:90:MET:CE	14:A3:808:CLA:HED2	2.31	0.61
14:A4:818:CLA:HMB1	14:A4:818:CLA:HBB1	1.82	0.61
1:A4:682:ILE:HD11	16:A4:849:BCR:C14	2.30	0.61
2:B1:53:LEU:CD1	14:B1:807:CLA:O1A	2.47	0.61
2:B2:532:GLY:HA2	2:B2:588:TRP:HZ3	1.65	0.61
2:B4:208:TRP:CH2	14:B4:816:CLA:H51	2.35	0.61
2:B6:532:GLY:HA2	2:B6:588:TRP:CZ3	2.36	0.61
2:B6:318:PHE:HA	14:B6:822:CLA:CAB	2.31	0.61
12:X6:9:TYR:O	12:X6:10:ALA:HB2	2.00	0.61
1:A2:177:TRP:HB2	14:A2:1613:CLA:HMC3	1.81	0.61
1:A2:440:ILE:HD11	14:A2:1633:CLA:NC	2.16	0.61
14:A4:827:CLA:H93	16:J4:103:BCR:H361	1.81	0.61
2:B2:503:TRP:CE3	14:B2:816:CLA:H11	2.36	0.61
2:B3:480:LEU:C	2:B3:482:SER:H	2.03	0.61
1:A6:587:CYS:O	2:B6:675:GLY:HA3	2.01	0.61
2:B6:144:LEU:HD21	14:B6:814:CLA:H152	1.81	0.61
14:A5:837:CLA:H101	14:L5:205:CLA:H191	1.83	0.61
1:A3:86:TRP:HA	14:A3:807:CLA:CBB	2.31	0.61
2:B1:275:HIS:HA	14:B1:818:CLA:C4B	2.31	0.61
2:B2:61:SER:OG	2:B2:138:ALA:O	2.19	0.61
2:B2:173:ARG:NE	14:B2:823:CLA:HMD1	2.16	0.61
2:B4:58:LEU:O	14:B4:809:CLA:CBB	2.49	0.61
2:B4:192:HIS:HB2	14:B4:816:CLA:C4B	2.30	0.61
9:K4:32:TYR:O	9:K4:34:ILE:N	2.34	0.61
1:A1:443:HIS:CD2	14:A1:830:CLA:HMB1	2.36	0.60
1:A5:84:PHE:CE1	14:A5:805:CLA:H91	2.36	0.60
2:B1:664:ALA:C	14:B1:806:CLA:HBB1	2.21	0.60
14:B1:854:CLA:HBA1	10:L2:148:ILE:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B5:41:LEU:O	2:B5:45:ILE:HG12	2.01	0.60
2:B6:532:GLY:HA2	2:B6:588:TRP:HZ3	1.66	0.60
7:I3:30:LEU:HD13	16:L3:206:BCR:HC8	1.83	0.60
1:A4:86:TRP:HA	14:A4:806:CLA:CBB	2.31	0.60
2:B1:457:LEU:HD22	2:B1:620:THR:HG21	1.84	0.60
2:B1:622:LEU:CD1	14:B1:805:CLA:C1	2.65	0.60
14:B1:820:CLA:HMD1	14:B1:822:CLA:HBB1	1.83	0.60
14:B2:818:CLA:HMD1	14:B2:820:CLA:HBB1	1.83	0.60
2:B3:216:PRO:HD3	14:B3:1817:CLA:O2D	2.01	0.60
12:X4:12:ARG:HB3	17:X4:101:LHG:HC5	1.83	0.60
1:A1:303:ALA:HB2	14:A1:817:CLA:HBB1	1.82	0.60
1:A2:453:PHE:CE1	14:B2:803:CLA:H12	2.36	0.60
1:A3:303:ALA:CB	14:A3:818:CLA:HBB1	2.30	0.60
14:A4:853:CLA:HMD2	10:L4:21:ILE:HD11	1.83	0.60
14:A6:1603:CLA:H71	14:A6:1640:CLA:HMC3	1.82	0.60
16:L3:201:BCR:H12C	14:L3:203:CLA:H42	1.81	0.60
14:L4:205:CLA:C9	14:B5:1812:CLA:H91	2.31	0.60
1:A3:281:PHE:HE1	14:A3:818:CLA:HAB	1.66	0.60
1:A3:352:TRP:NE1	14:A3:825:CLA:H191	2.17	0.60
2:B1:177:HIS:CB	14:B1:825:CLA:HED3	2.30	0.60
2:B5:261:HIS:HD2	2:B5:263:GLN:H	1.46	0.60
14:A6:1602:CLA:HAB	14:B6:804:CLA:NA	2.17	0.60
14:B6:819:CLA:HMD1	14:B6:821:CLA:HBB1	1.83	0.60
5:E2:39:ARG:NH1	13:P2:24:TYR:CZ	2.68	0.60
8:J1:31:ARG:HD3	16:J1:104:BCR:H312	1.82	0.60
14:L4:205:CLA:H91	14:B5:1812:CLA:H101	1.84	0.60
14:A6:1601:CLA:HAC2	14:L6:207:CLA:H151	1.83	0.60
2:B2:592:THR:O	2:B2:596:VAL:HG13	2.02	0.60
2:B2:256:PHE:HB2	14:B2:815:CLA:O1D	2.02	0.60
2:B3:122:TRP:HH2	16:B3:1847:BCR:H391	1.64	0.60
2:B3:65:PHE:CZ	14:B3:1809:CLA:HAC2	2.37	0.60
2:B5:344:LEU:O	2:B5:348:THR:OG1	2.18	0.60
2:B6:144:LEU:CD2	14:B6:814:CLA:H152	2.31	0.60
10:L5:142:PHE:HB2	14:L5:206:CLA:H43	1.83	0.60
1:A1:651:ARG:NE	1:A1:652:ASP:OD2	2.33	0.60
14:A2:1602:CLA:HAB	14:B2:801:CLA:NA	2.17	0.60
1:A4:592:TRP:NE1	14:A4:829:CLA:HMD1	2.16	0.60
1:A5:28:TRP:HZ2	14:A5:804:CLA:H11	1.66	0.60
1:A6:79:HIS:CD2	14:A6:1605:CLA:HMA1	2.37	0.60
2:B3:344:LEU:HD22	14:B3:1807:CLA:HED3	1.82	0.60
14:B3:1821:CLA:HMD1	14:B3:1823:CLA:HBB1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:188:ALA:HB2	14:B3:1830:CLA:H202	1.82	0.60
14:B3:1834:CLA:HBB1	14:B3:1835:CLA:HMB2	1.84	0.60
2:B4:637:LEU:HD22	2:B4:730:PHE:HA	1.84	0.60
2:B4:498:VAL:HG11	14:B4:818:CLA:HED2	1.84	0.60
2:B4:514:LEU:CD1	14:B4:828:CLA:CMC	2.80	0.60
2:B6:114:ILE:O	14:B6:808:CLA:HMD3	2.01	0.60
1:A3:435:ARG:HD2	4:D3:12:GLY:O	2.01	0.60
1:A4:718:GLN:NE2	5:E4:15:TYR:OH	2.35	0.60
9:K3:32:TYR:O	9:K3:34:ILE:N	2.34	0.60
10:L2:105:GLY:O	10:L2:106:SER:HB2	2.00	0.60
1:A6:270:PHE:CD1	14:A6:1641:CLA:HMD2	2.37	0.60
1:A6:323:HIS:HB3	1:A6:328:ILE:HD11	1.84	0.60
2:B3:41:LEU:O	2:B3:45:ILE:HG12	2.02	0.60
2:B4:591:ASN:HB2	14:B4:804:CLA:HBC2	1.82	0.60
9:K2:32:TYR:O	9:K2:34:ILE:N	2.35	0.60
12:X2:9:TYR:O	12:X2:10:ALA:HB2	2.01	0.60
2:B5:318:PHE:HB2	14:B5:1825:CLA:HMA1	1.84	0.60
6:F4:73:ILE:O	6:F4:76:TRP:HB3	2.01	0.60
1:A5:305:ALA:O	1:A5:309:ILE:HG12	2.01	0.60
14:A6:1619:CLA:HBB1	14:A6:1619:CLA:HMB1	1.83	0.60
2:B1:267:LEU:HD22	14:B1:818:CLA:HBA1	1.84	0.60
2:B1:52:HIS:ND1	14:B1:807:CLA:CMA	2.65	0.60
2:B1:64:LEU:HD11	16:B1:845:BCR:H271	1.84	0.60
2:B2:318:PHE:H	14:B2:821:CLA:C2B	2.14	0.60
2:B3:195:HIS:CG	14:B3:1816:CLA:CBC	2.85	0.60
6:F2:70:PHE:HD1	16:F2:201:BCR:H321	1.67	0.60
10:L1:39:GLN:HA	10:L1:39:GLN:OE1	2.00	0.60
3:C3:11:ILE:CD1	13:P3:39:SER:C	2.70	0.60
12:X4:9:TYR:O	12:X4:10:ALA:HB2	2.01	0.60
14:A5:843:CLA:HAA2	14:L5:202:CLA:HAA2	1.82	0.60
1:A6:683:TRP:O	1:A6:686:SER:OG	2.19	0.60
2:B1:379:GLN:OE1	14:B1:826:CLA:HMD1	2.01	0.60
2:B2:116:TYR:HA	2:B2:370:THR:HG22	1.84	0.60
14:B2:818:CLA:HAA2	14:B2:823:CLA:HBB1	1.84	0.60
14:B4:821:CLA:HMD1	14:B4:823:CLA:HBB1	1.84	0.60
14:B5:1839:CLA:HMB2	14:B5:1841:CLA:HED1	1.82	0.60
2:B5:727:TYR:HB2	14:B5:1803:CLA:HED3	1.83	0.60
11:M4:9:TYR:CB	16:M4:101:BCR:H401	2.31	0.60
1:A3:180:TYR:CE2	14:A3:811:CLA:C4D	2.85	0.59
1:A3:429:VAL:O	1:A3:433:VAL:HG13	2.02	0.59
2:B2:41:LEU:O	2:B2:45:ILE:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:216:PRO:HD2	14:B3:1817:CLA:C3D	2.32	0.59
2:B3:431:PHE:CZ	16:B3:1851:BCR:HC41	2.36	0.59
2:B3:447:VAL:HG11	2:B3:621:TYR:CZ	2.36	0.59
2:B4:400:ASP:OD1	4:D4:129:LYS:NZ	2.35	0.59
2:B6:446:VAL:HG13	2:B6:451:THR:O	2.01	0.59
14:B6:832:CLA:HBB1	14:B6:833:CLA:HMB2	1.84	0.59
11:M6:29:LEU:O	11:M6:30:TYR:HB2	2.02	0.59
1:A1:706:TRP:CG	2:B1:419:GLU:HG3	2.37	0.59
1:A4:651:ARG:HB2	2:B4:638:ILE:HG23	1.83	0.59
1:A4:683:TRP:O	1:A4:686:SER:OG	2.20	0.59
1:A5:19:ASP:HA	1:A5:181:HIS:O	2.03	0.59
14:B2:822:CLA:HBB1	14:B2:829:CLA:HMD2	1.84	0.59
14:B3:1832:CLA:HBC1	16:B3:1848:BCR:H23C	1.84	0.59
2:B4:354:HIS:ND1	14:B4:819:CLA:OBD	2.35	0.59
2:B5:440:TYR:CZ	2:B5:524:LEU:HB3	2.37	0.59
5:E5:54:GLY:O	5:E5:55:VAL:O	2.19	0.59
12:X4:26:VAL:CG1	14:X4:102:CLA:HED3	2.32	0.59
1:A1:682:ILE:HD12	16:A1:847:BCR:C35	2.32	0.59
1:A5:302:LEU:HD13	14:A5:815:CLA:HMC1	1.84	0.59
14:A6:1626:CLA:HAA2	14:A6:1627:CLA:OBD	2.02	0.59
2:B4:281:VAL:HG13	16:B4:845:BCR:H351	1.83	0.59
2:B5:718:HIS:HE1	14:B5:1843:CLA:C4D	2.15	0.59
14:B2:808:CLA:H201	7:I2:23:PRO:HA	1.85	0.59
7:I3:20:TRP:NE1	16:I3:102:BCR:HC22	2.16	0.59
9:K1:73:VAL:HA	14:K1:1401:CLA:CBB	2.20	0.59
1:A1:40:ARG:NE	13:P1:61:ASP:HA	2.17	0.59
1:A2:603:TYR:OH	14:A2:1602:CLA:HBA1	2.03	0.59
1:A6:207:LEU:HD21	14:A6:1620:CLA:HMC1	1.84	0.59
2:B1:300:ILE:HG21	14:B1:825:CLA:HMC1	1.83	0.59
14:B1:831:CLA:HBC1	16:B1:846:BCR:H23C	1.84	0.59
2:B6:642:ASN:HB2	2:B6:643:PRO:CD	2.31	0.59
7:I1:30:LEU:HD13	16:I1:103:BCR:C8	2.33	0.59
10:L6:105:GLY:O	10:L6:106:SER:HB2	2.01	0.59
12:X1:9:TYR:O	12:X1:10:ALA:HB2	2.02	0.59
1:A3:444:LEU:HD13	14:A3:839:CLA:C3B	2.32	0.59
1:A4:233:ALA:O	1:A4:235:ASP:N	2.36	0.59
2:B1:229:TRP:CZ2	14:B1:817:CLA:H71	2.37	0.59
2:B1:256:PHE:HZ	14:B1:818:CLA:H112	1.67	0.59
2:B1:59:TRP:CG	14:B1:808:CLA:HBC1	2.37	0.59
14:B6:807:CLA:H102	14:B6:807:CLA:H151	1.84	0.59
3:C2:30:TRP:O	3:C2:36:GLY:HA2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:682:ILE:HD11	16:A1:847:BCR:C13	2.33	0.59
1:A6:303:ALA:HB2	14:A6:1618:CLA:HBB1	1.83	0.59
2:B1:334:HIS:HE1	14:B1:830:CLA:HED1	1.67	0.59
2:B1:503:TRP:NE1	14:B1:835:CLA:HED1	2.17	0.59
14:B4:834:CLA:HBB1	14:B4:835:CLA:HMB2	1.85	0.59
14:B6:830:CLA:HBC1	16:B6:846:BCR:H23C	1.84	0.59
3:C5:62:LEU:HD12	3:C5:65:ARG:NE	2.17	0.59
1:A3:308:PHE:HE2	14:A3:821:CLA:HAB	1.67	0.59
1:A4:612:HIS:CE1	14:A4:835:CLA:C2C	2.86	0.59
1:A4:675:LEU:HD11	14:A4:827:CLA:H143	1.83	0.59
14:A4:825:CLA:HAA2	14:A4:826:CLA:OBD	2.03	0.59
1:A6:489:TRP:O	1:A6:493:LEU:HG	2.03	0.59
2:B2:141:LEU:HD23	2:B2:144:LEU:HD12	1.84	0.59
14:B2:831:CLA:HBB1	14:B2:832:CLA:HMB2	1.85	0.59
2:B4:189:TRP:N	14:B4:816:CLA:CBB	2.66	0.59
2:B5:153:TRP:CZ3	14:B5:1801:CLA:C6	2.81	0.59
2:B6:188:ALA:HA	14:B6:815:CLA:HBB2	1.85	0.59
14:A1:825:CLA:HAA2	14:A1:826:CLA:OBD	2.03	0.59
1:A5:86:TRP:HA	14:A5:807:CLA:CBB	2.33	0.59
1:A6:429:VAL:O	1:A6:433:VAL:HG13	2.01	0.59
14:B2:805:CLA:H162	14:B2:827:CLA:HBB2	1.85	0.59
2:B3:50:PHE:CD1	2:B3:152:GLY:HA2	2.38	0.59
2:B3:493:PRO:HG3	14:B3:1838:CLA:ND	2.17	0.59
2:B3:414:VAL:HG11	16:B3:1848:BCR:H401	1.83	0.59
2:B4:174:LEU:HD21	14:B4:826:CLA:C4D	2.33	0.59
2:B4:304:MET:HG3	2:B4:322:HIS:O	2.03	0.59
2:B4:711:ALA:CB	15:B4:844:PQN:C8	2.81	0.59
1:A4:456:PHE:CE2	14:B4:805:CLA:H92	2.38	0.59
2:B4:229:TRP:CE3	14:B4:818:CLA:C2B	2.85	0.59
2:B6:41:LEU:O	2:B6:45:ILE:HG12	2.02	0.59
5:E4:57:THR:HG23	13:P4:42:ALA:HB1	1.78	0.59
6:F4:103:VAL:HB	6:F4:104:PRO:HD3	1.84	0.59
8:J1:27:ILE:CG2	16:J1:104:BCR:C34	2.79	0.59
14:L1:201:CLA:H12	14:L1:206:CLA:H93	1.85	0.59
16:I1:103:BCR:H401	10:L1:89:ALA:HB1	1.85	0.59
10:L2:146:ASP:O	10:L2:150:THR:HG23	2.02	0.59
14:A2:1634:CLA:H143	16:L2:201:BCR:H313	1.85	0.59
1:A6:86:TRP:HA	14:A6:1607:CLA:CBB	2.33	0.59
1:A6:19:ASP:HA	1:A6:181:HIS:O	2.03	0.59
2:B3:281:VAL:HG22	16:B3:1845:BCR:H352	1.85	0.59
2:B4:525:VAL:HG12	14:B4:803:CLA:C14	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B4:832:CLA:HBC1	16:B4:848:BCR:H23C	1.84	0.59
8:J6:13:VAL:HA	16:J6:1105:BCR:H401	1.85	0.59
1:A4:453:PHE:O	14:L4:201:CLA:CBB	2.50	0.59
16:L5:201:BCR:H12C	14:L5:204:CLA:H42	1.83	0.59
5:E5:39:ARG:NH2	13:P5:24:TYR:CZ	2.63	0.59
1:A1:303:ALA:CB	14:A1:817:CLA:HBB1	2.32	0.59
1:A2:582:GLY:HA3	3:C2:48:VAL:O	2.03	0.59
14:A4:822:CLA:HMA1	14:B5:1801:CLA:HAC2	1.85	0.59
1:A5:744:TRP:CH2	14:A5:828:CLA:H43	2.37	0.59
2:B1:230:GLY:CA	14:B1:817:CLA:HBA1	2.33	0.59
2:B1:286:ALA:HB2	14:B1:820:CLA:C3C	2.32	0.59
2:B1:229:TRP:CB	14:B1:817:CLA:HBA2	2.33	0.59
2:B1:358:LEU:HD11	14:B1:827:CLA:HHC	1.85	0.59
2:B4:48:SER:HB3	14:B4:807:CLA:HBB1	1.85	0.59
14:B5:1832:CLA:HBC1	16:B5:1848:BCR:H23C	1.84	0.59
14:B6:841:CLA:H151	10:L6:92:CYS:SG	2.43	0.59
5:E2:57:THR:HG21	13:P2:42:ALA:HA	1.85	0.59
8:J4:31:ARG:CZ	14:J4:101:CLA:HED2	2.32	0.59
10:L5:48:LEU:CD1	14:L5:204:CLA:CED	2.81	0.59
14:B1:853:CLA:HAC2	14:A2:1625:CLA:HMA1	1.85	0.58
14:A2:1635:CLA:C3B	14:L2:202:CLA:HMB2	2.33	0.58
14:A3:834:CLA:O1A	10:L3:62:TRP:CD1	2.56	0.58
14:A4:841:CLA:H192	10:L4:58:LEU:CD2	2.33	0.58
14:B1:833:CLA:HBB1	14:B1:834:CLA:HMB2	1.84	0.58
14:A1:822:CLA:HMA1	14:B3:1801:CLA:HAC2	1.84	0.58
7:I4:25:VAL:HG13	14:L6:206:CLA:H111	1.85	0.58
10:L3:105:GLY:O	10:L3:106:SER:HB2	2.03	0.58
1:A1:305:ALA:O	1:A1:309:ILE:HG12	2.03	0.58
1:A1:682:ILE:CD1	16:A1:847:BCR:C35	2.81	0.58
1:A1:86:TRP:HA	14:A1:806:CLA:CBB	2.33	0.58
1:A2:19:ASP:HA	1:A2:181:HIS:O	2.03	0.58
1:A4:221:LEU:HB2	1:A4:222:PRO:HD3	1.84	0.58
1:A6:83:VAL:HG11	14:A6:1605:CLA:H72	1.85	0.58
2:B1:660:HIS:CD2	14:B1:804:CLA:C1B	2.87	0.58
14:B2:840:CLA:H151	10:L2:92:CYS:SG	2.44	0.58
14:B2:829:CLA:HBC1	16:B2:845:BCR:H23C	1.84	0.58
2:B3:122:TRP:CH2	16:B3:1847:BCR:H391	2.38	0.58
14:B3:1808:CLA:H143	14:B3:1830:CLA:HBB2	1.85	0.58
2:B3:281:VAL:HG13	16:B3:1845:BCR:C35	2.32	0.58
2:B3:493:PRO:HG3	14:B3:1838:CLA:C3D	2.33	0.58
2:B3:90:ILE:HB	2:B3:111:PRO:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B5:1821:CLA:HMD1	14:B5:1823:CLA:HBB1	1.84	0.58
1:A5:587:CYS:HB2	2:B5:673:TRP:CB	2.33	0.58
2:B6:630:LEU:CD1	14:B6:804:CLA:H93	2.33	0.58
10:L2:54:HIS:O	10:L2:58:LEU:HG	2.03	0.58
14:A4:832:CLA:C3B	14:L4:201:CLA:HMB2	2.33	0.58
12:X3:12:ARG:CB	17:X3:101:LHG:HC5	2.30	0.58
1:A5:399:TRP:CD1	14:A5:828:CLA:HAB	2.37	0.58
2:B1:286:ALA:HB2	14:B1:820:CLA:C2C	2.33	0.58
2:B2:114:ILE:O	14:B2:807:CLA:HMD3	2.03	0.58
7:I2:22:MET:HE2	16:I2:101:BCR:H331	1.85	0.58
10:L1:134:VAL:CB	16:L1:209:BCR:H403	2.32	0.58
14:B6:810:CLA:HMA2	10:L5:148:ILE:HG23	1.83	0.58
1:A1:207:LEU:HD13	16:A1:843:BCR:C36	2.34	0.58
1:A1:341:HIS:HE1	17:A1:849:LHG:HC11	1.67	0.58
1:A4:305:ALA:O	1:A4:309:ILE:HG12	2.04	0.58
1:A4:313:HIS:CE1	16:A4:844:BCR:H363	2.39	0.58
1:A5:360:LEU:HD13	14:A5:830:CLA:HBB1	1.84	0.58
2:B1:339:TRP:CZ3	16:B1:846:BCR:H372	2.38	0.58
2:B1:664:ALA:HB2	14:B1:801:CLA:C3D	2.33	0.58
2:B4:294:PHE:HE1	14:B4:814:CLA:HMA1	1.68	0.58
14:B5:1834:CLA:HBB1	14:B5:1835:CLA:HMB2	1.85	0.58
14:B6:823:CLA:HBB1	14:B6:830:CLA:HMD2	1.84	0.58
14:B6:819:CLA:CMB	14:B6:824:CLA:HMA3	2.33	0.58
3:C2:62:LEU:HD12	3:C2:65:ARG:NE	2.17	0.58
6:F6:24:THR:OG1	6:F6:34:ARG:NH1	2.36	0.58
14:B1:854:CLA:CMB	7:I1:20:TRP:HZ2	2.09	0.58
7:I2:7:ALA:N	11:M2:5:ASP:OD1	2.36	0.58
1:A1:602:MET:HG2	14:A1:825:CLA:HBC1	1.85	0.58
1:A2:681:PHE:CG	16:A2:1652:BCR:H363	2.39	0.58
1:A3:19:ASP:HA	1:A3:181:HIS:O	2.02	0.58
14:A3:843:CLA:H192	10:L3:58:LEU:HD21	1.86	0.58
1:A4:612:HIS:ND1	14:A4:835:CLA:HMC2	2.17	0.58
14:B1:808:CLA:H162	14:B1:829:CLA:HBB2	1.85	0.58
2:B3:281:VAL:HG13	16:B3:1845:BCR:H351	1.86	0.58
2:B4:554:PRO:HD2	3:C4:61:PHE:CZ	2.39	0.58
2:B4:174:LEU:HD21	14:B4:826:CLA:C2D	2.34	0.58
14:B4:821:CLA:CMB	14:B4:826:CLA:HMA3	2.34	0.58
14:B6:807:CLA:H143	14:B6:828:CLA:HBB2	1.86	0.58
6:F1:65:ILE:CD1	14:J1:102:CLA:HMB3	2.32	0.58
10:L6:115:GLU:O	10:L6:118:SER:OG	2.17	0.58
5:E4:57:THR:CG2	13:P4:42:ALA:HB1	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A2:1644:CLA:HMA1	2:B2:694:ALA:HB1	1.85	0.58
14:A4:853:CLA:HBD	14:B5:1801:CLA:HMA2	1.85	0.58
2:B1:339:TRP:CH2	14:B1:824:CLA:HBC2	2.39	0.58
2:B1:685:VAL:HG21	3:C1:80:TYR:CE1	2.39	0.58
2:B2:261:HIS:HD2	2:B2:263:GLN:H	1.51	0.58
2:B3:599:TYR:CE2	14:B3:1839:CLA:C2C	2.86	0.58
2:B4:521:GLY:CA	2:B4:619:SER:OG	2.51	0.58
2:B5:599:TYR:CE2	14:B5:1839:CLA:C2C	2.87	0.58
14:B2:808:CLA:H203	7:I2:26:VAL:CG2	2.32	0.58
8:J6:26:LEU:HD23	16:J6:1104:BCR:C7	2.32	0.58
1:A2:688:MET:O	1:A2:692:SER:OG	2.20	0.58
14:A5:823:CLA:HMA1	14:A5:843:CLA:HAC2	1.85	0.58
1:A6:305:ALA:O	1:A6:309:ILE:HG12	2.04	0.58
2:B4:189:TRP:N	14:B4:816:CLA:HBB1	2.19	0.58
14:A6:1603:CLA:HBA2	2:B6:430:LEU:HD12	1.86	0.58
1:A4:683:TRP:NE1	14:A4:801:CLA:HBA2	2.19	0.58
14:B2:818:CLA:CMB	14:B2:823:CLA:HMA3	2.34	0.58
2:B2:600:TRP:HB2	14:B2:836:CLA:HMC1	1.84	0.58
14:A3:801:CLA:HAB	14:B3:1803:CLA:NA	2.19	0.58
2:B3:195:HIS:ND1	14:B3:1816:CLA:CBC	2.67	0.58
2:B3:672:SER:HG	2:B3:677:TRP:HE1	1.49	0.58
2:B5:377:HIS:HE2	14:B5:1830:CLA:C1B	2.17	0.58
14:B5:1808:CLA:H162	14:B5:1830:CLA:HBB2	1.86	0.58
2:B5:625:TRP:CZ2	14:B5:1803:CLA:H142	2.38	0.58
14:A2:1634:CLA:H12	14:L2:206:CLA:H93	1.86	0.58
14:A5:842:CLA:H151	10:L5:85:LEU:HD22	1.85	0.58
1:A6:84:PHE:CZ	14:A6:1605:CLA:H91	2.38	0.58
1:A6:90:MET:HE2	14:A6:1628:CLA:HED1	1.85	0.58
2:B2:446:VAL:HG13	2:B2:451:THR:O	2.04	0.58
2:B2:52:HIS:CE1	14:B2:804:CLA:HMA2	2.39	0.58
2:B2:493:PRO:HG3	14:B2:835:CLA:C1D	2.34	0.58
2:B3:481:LEU:HD11	14:B3:1836:CLA:CAD	2.34	0.58
2:B4:174:LEU:HD21	14:B4:826:CLA:ND	2.18	0.58
6:F5:76:TRP:CZ3	14:F5:1301:CLA:HBA2	2.39	0.58
6:F6:76:TRP:CE3	14:F6:202:CLA:HBA2	2.38	0.58
7:I1:30:LEU:HD13	16:I1:103:BCR:C6	2.33	0.58
1:A2:233:ALA:O	1:A2:235:ASP:N	2.37	0.58
1:A4:259:GLY:O	1:A4:261:PHE:N	2.37	0.58
1:A5:744:TRP:CZ2	14:A5:828:CLA:H43	2.38	0.58
1:A6:352:TRP:NE1	14:A6:1625:CLA:H191	2.18	0.58
2:B1:11:LEU:HD11	2:B1:26:MET:SD	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B1:828:CLA:HBC3	19:B1:850:LMG:H421	1.86	0.58
2:B3:724:ILE:HD13	19:B3:1850:LMG:H431	1.84	0.58
2:B4:181:LEU:HD13	14:B4:815:CLA:HBB	1.86	0.58
7:I4:27:MET:SD	16:L4:206:BCR:H352	2.44	0.58
1:A1:31:PRO:HB3	14:A1:802:CLA:HAC1	1.84	0.57
1:A2:269:THR:O	1:A2:270:PHE:HB2	2.04	0.57
14:B1:808:CLA:H143	14:B1:829:CLA:HBB2	1.86	0.57
2:B2:339:TRP:CZ2	14:B2:823:CLA:CAB	2.86	0.57
2:B2:229:TRP:CB	14:B2:815:CLA:H12	2.22	0.57
2:B3:288:HIS:O	14:B3:1822:CLA:HED1	2.04	0.57
2:B3:398:VAL:CG2	2:B3:547:ALA:HB1	2.34	0.57
2:B4:350:LEU:HD23	14:B4:820:CLA:H62	1.86	0.57
14:B5:1821:CLA:CMB	14:B5:1826:CLA:HMA3	2.34	0.57
14:B5:1835:CLA:O1D	8:J5:35:ASP:HA	2.04	0.57
1:A1:604:ASN:HD21	14:A1:801:CLA:H201	1.69	0.57
14:A5:801:CLA:HAB	14:B5:1803:CLA:NA	2.18	0.57
2:B3:174:LEU:HD21	14:B3:1826:CLA:C1D	2.34	0.57
2:B3:59:TRP:HA	14:B3:1809:CLA:HBB2	1.86	0.57
2:B6:52:HIS:CE1	14:B6:806:CLA:HMA2	2.39	0.57
14:B6:807:CLA:H162	14:B6:828:CLA:HBB2	1.85	0.57
8:J1:32:PHE:HE1	14:J1:101:CLA:HMA3	1.68	0.57
14:A3:843:CLA:H151	10:L3:85:LEU:CD2	2.34	0.57
10:L4:7:PRO:HB3	10:L4:12:PRO:HA	1.85	0.57
10:L6:129:MET:SD	16:L5:201:BCR:H24C	2.45	0.57
10:L6:33:ASN:O	10:L6:38:ARG:NE	2.24	0.57
11:M3:12:LEU:HB3	16:M3:1602:BCR:C21	2.35	0.57
11:M3:9:TYR:CB	16:M3:1602:BCR:H401	2.28	0.57
1:A2:40:ARG:NH1	13:P2:62:GLN:O	2.37	0.57
1:A3:646:ILE:HG13	14:A3:802:CLA:H12	1.85	0.57
14:A4:831:CLA:H12	14:L4:204:CLA:H93	1.86	0.57
1:A4:341:HIS:HE1	17:A4:851:LHG:HC11	1.69	0.57
1:A6:259:GLY:O	1:A6:261:PHE:N	2.38	0.57
2:B1:444:ASP:OD2	2:B1:622:LEU:N	2.34	0.57
14:B4:808:CLA:H162	14:B4:830:CLA:HBB2	1.86	0.57
2:B4:493:PRO:HG3	14:B4:838:CLA:C4D	2.34	0.57
2:B5:166:TRP:CZ2	14:B5:1815:CLA:HAC2	2.40	0.57
8:J1:27:ILE:HG21	16:J1:104:BCR:H343	1.82	0.57
11:M6:4:THR:N	11:M6:7:GLN:OE1	2.31	0.57
12:X4:23:ASN:OD1	14:X4:102:CLA:C4A	2.52	0.57
14:A3:802:CLA:H41	2:B3:654:TRP:CD1	2.38	0.57
14:A3:833:CLA:C3B	14:A3:834:CLA:HMB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:691:PHE:O	2:B4:583:TYR:OH	2.17	0.57
1:A5:90:MET:CE	14:A5:828:CLA:HED1	2.33	0.57
14:A5:842:CLA:H191	14:L5:205:CLA:HBB1	1.85	0.57
2:B1:466:ILE:HD12	14:B1:838:CLA:CGA	2.35	0.57
14:B2:805:CLA:H143	14:B2:827:CLA:HBB2	1.86	0.57
2:B5:386:MET:HE1	16:B5:1849:BCR:C36	2.33	0.57
1:A4:581:PRO:HG2	3:C4:68:LEU:HD11	1.85	0.57
5:E6:24:ALA:O	5:E6:25:SER:HB3	2.04	0.57
6:F4:70:PHE:HB2	16:F4:201:BCR:H321	1.84	0.57
5:E2:57:THR:CG2	13:P2:42:ALA:HB2	2.34	0.57
12:X2:23:ASN:OD1	14:X2:1701:CLA:CHB	2.52	0.57
1:A1:90:MET:HE3	14:A1:807:CLA:HED2	1.87	0.57
1:A3:281:PHE:CE1	14:A3:818:CLA:HAB	2.40	0.57
14:A3:826:CLA:HAA2	14:A3:827:CLA:OBD	2.04	0.57
14:A3:843:CLA:H191	14:L3:204:CLA:HBB1	1.87	0.57
14:A5:826:CLA:HAA2	14:A5:827:CLA:OBD	2.05	0.57
1:A6:682:ILE:HD11	16:A6:1648:BCR:C14	2.35	0.57
14:B3:1808:CLA:H162	14:B3:1830:CLA:HBB2	1.86	0.57
2:B4:398:VAL:CG2	2:B4:547:ALA:HB1	2.35	0.57
2:B5:153:TRP:CH2	14:B5:1801:CLA:H62	2.39	0.57
2:B5:466:ILE:CD1	14:B5:1839:CLA:O2A	2.52	0.57
14:A4:841:CLA:H191	14:L4:204:CLA:HBB1	1.86	0.57
10:L5:62:TRP:CZ2	14:L5:203:CLA:H11	2.39	0.57
14:A2:1644:CLA:H191	14:L2:206:CLA:HBB1	1.86	0.57
1:A4:83:VAL:HG11	14:A4:804:CLA:H72	1.85	0.57
1:A5:352:TRP:CZ3	14:A5:825:CLA:H112	2.39	0.57
1:A6:303:ALA:CB	14:A6:1618:CLA:HBB1	2.33	0.57
1:A6:233:ALA:O	1:A6:235:ASP:N	2.36	0.57
1:A6:646:ILE:HD11	14:A6:1602:CLA:H151	1.85	0.57
14:B3:1835:CLA:H11	8:J3:29:PHE:CE2	2.39	0.57
2:B3:195:HIS:ND1	14:B3:1816:CLA:HBC1	2.19	0.57
2:B4:182:PHE:CE1	14:B4:826:CLA:HED2	2.39	0.57
14:B4:808:CLA:H143	14:B4:830:CLA:HBB2	1.86	0.57
2:B4:122:TRP:CH2	16:B4:847:BCR:H391	2.40	0.57
14:B4:829:CLA:HBC3	19:B4:851:LMG:H421	1.87	0.57
14:B4:852:CLA:HAC2	14:A6:1623:CLA:HMA1	1.85	0.57
14:B4:852:CLA:HBA1	14:A6:1601:CLA:HAA2	1.87	0.57
2:B5:150:PHE:HZ	14:B5:1801:CLA:C2	2.17	0.57
2:B5:525:VAL:HG12	14:B5:1803:CLA:C14	2.30	0.57
1:A6:468:PHE:CZ	14:B6:809:CLA:CHC	2.88	0.57
6:F4:53:VAL:HG12	6:F4:63:PHE:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L3:41:LEU:HD13	10:L3:45:LEU:HD23	1.87	0.57
10:L6:21:ILE:HB	14:L6:202:CLA:CAD	2.35	0.57
11:M2:29:LEU:O	11:M2:30:TYR:HB2	2.04	0.57
1:A1:453:PHE:O	14:L1:202:CLA:CBB	2.53	0.57
14:A2:1628:CLA:HAA2	14:A2:1629:CLA:OBD	2.04	0.57
14:A3:823:CLA:HMA1	14:A3:845:CLA:HAC2	1.85	0.57
1:A4:36:ARG:HH12	13:P4:71:GLU:HG3	1.70	0.57
16:A5:850:BCR:H23C	16:A5:850:BCR:H403	1.86	0.57
2:B1:182:PHE:CE1	14:B1:825:CLA:HED2	2.40	0.57
2:B3:493:PRO:HG3	14:B3:1838:CLA:C2D	2.34	0.57
2:B3:480:LEU:O	2:B3:482:SER:N	2.38	0.57
1:A4:464:THR:HG1	2:B4:654:TRP:HE1	1.53	0.57
2:B5:402:ASP:O	2:B5:406:ASN:OD1	2.23	0.57
2:B5:497:ASN:O	2:B5:498:VAL:HB	2.04	0.57
2:B6:339:TRP:HZ2	14:B6:824:CLA:HAB	1.70	0.57
8:J5:27:ILE:CD1	16:J5:104:BCR:C11	2.82	0.57
14:A1:839:CLA:H191	14:L1:206:CLA:HBB1	1.85	0.57
1:A1:578:CYS:SG	18:A1:850:SF4:S1	3.02	0.57
16:A2:1652:BCR:H403	16:A2:1652:BCR:H23C	1.86	0.57
1:A3:40:ARG:HD3	13:P3:61:ASP:HA	1.87	0.57
1:A3:587:CYS:HG	18:A3:855:SF4:FE2	1.22	0.57
1:A4:177:TRP:HB2	14:A4:810:CLA:HMC3	1.87	0.57
1:A4:682:ILE:HD12	16:A4:849:BCR:C35	2.35	0.57
1:A6:578:CYS:HB3	1:A6:587:CYS:HA	1.87	0.57
2:B2:586:MET:HG3	2:B2:716:LEU:HD21	1.86	0.57
1:A4:466:ARG:O	2:B4:646:THR:HG21	2.04	0.57
2:B4:207:GLY:HA2	14:B4:816:CLA:OBD	2.05	0.57
14:B6:810:CLA:C4	10:L6:81:SER:HA	2.35	0.57
6:F4:76:TRP:NE1	14:F4:202:CLA:HBD	2.19	0.57
1:A2:544:PHE:HZ	14:A2:1603:CLA:CBB	2.18	0.57
14:B1:820:CLA:CMB	14:B1:825:CLA:HMA3	2.35	0.57
14:B3:1821:CLA:CMB	14:B3:1826:CLA:HMA3	2.35	0.57
2:B4:61:SER:OG	2:B4:138:ALA:O	2.23	0.57
2:B4:192:HIS:HB2	14:B4:816:CLA:CHC	2.35	0.57
2:B4:456:ILE:HG22	2:B4:458:ILE:HD11	1.86	0.57
2:B5:731:LEU:HD22	14:B5:1829:CLA:HMB1	1.86	0.57
1:A5:555:LYS:HD3	2:B5:676:TYR:CE1	2.40	0.57
8:J6:13:VAL:HG22	16:J6:1105:BCR:H292	1.87	0.57
10:L5:116:GLY:O	10:L5:119:GLN:N	2.37	0.57
14:L6:203:CLA:H191	14:L6:207:CLA:HBB1	1.86	0.57
1:A3:221:LEU:HB2	1:A3:222:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A6:200:HIS:CE1	14:A6:1625:CLA:H52	2.40	0.57
2:B2:480:LEU:O	2:B2:482:SER:N	2.38	0.57
14:B5:1829:CLA:HBC3	19:B5:1851:LMG:H421	1.87	0.57
2:B5:731:LEU:HD22	14:B5:1829:CLA:CMB	2.35	0.57
2:B6:166:TRP:CZ2	14:B6:813:CLA:HAC2	2.40	0.57
3:C2:7:TYR:OH	3:C2:67:TYR:OH	2.20	0.57
10:L1:46:ARG:O	10:L1:50:VAL:HG23	2.05	0.57
1:A1:50:ASN:O	1:A1:51:LEU:C	2.44	0.56
14:A3:803:CLA:HED1	8:J3:12:PRO:HA	1.85	0.56
16:A3:852:BCR:H403	16:A3:852:BCR:H23C	1.85	0.56
2:B1:274:HIS:ND1	14:B1:818:CLA:HMB1	2.20	0.56
2:B1:189:TRP:CE3	14:B1:819:CLA:HMD3	2.40	0.56
2:B2:188:ALA:HA	14:B2:814:CLA:HBB2	1.86	0.56
2:B4:176:HIS:HB3	14:B4:815:CLA:CHC	2.35	0.56
2:B5:64:LEU:HD11	16:B5:1847:BCR:H271	1.87	0.56
2:B6:480:LEU:O	2:B6:482:SER:N	2.38	0.56
1:A1:423:ALA:HA	4:D1:38:VAL:HG11	1.87	0.56
1:A1:567:PRO:HD2	4:D1:62:GLU:CD	2.26	0.56
14:L6:202:CLA:H12	14:L6:207:CLA:H93	1.86	0.56
16:A1:847:BCR:H403	16:A1:847:BCR:H23C	1.86	0.56
1:A3:300:HIS:O	1:A3:304:ILE:HG12	2.05	0.56
1:A4:444:LEU:HB2	14:A4:837:CLA:CBB	2.34	0.56
14:A5:833:CLA:C3B	14:L5:203:CLA:HMB2	2.35	0.56
1:A5:697:TRP:CH2	15:A5:844:PQN:H2M3	2.40	0.56
2:B1:660:HIS:NE2	14:B1:804:CLA:C1B	2.68	0.56
2:B4:497:ASN:O	2:B4:498:VAL:HB	2.05	0.56
14:B4:808:CLA:H151	14:B4:808:CLA:H102	1.87	0.56
2:B5:537:THR:HG21	14:B5:1827:CLA:CBB	2.34	0.56
2:B6:372:ALA:HA	2:B6:600:TRP:CZ3	2.39	0.56
2:B6:52:HIS:NE2	14:B6:806:CLA:CMA	2.66	0.56
2:B6:340:HIS:CG	14:B6:824:CLA:HAA1	2.41	0.56
1:A1:47:TRP:HD1	5:E1:52:ALA:HB1	1.70	0.56
6:F1:53:VAL:HG12	6:F1:63:PHE:HB2	1.87	0.56
6:F1:65:ILE:HB	6:F1:66:PRO:HD3	1.87	0.56
14:B4:812:CLA:H52	7:I4:20:TRP:CH2	2.40	0.56
14:A1:831:CLA:C3B	14:L1:202:CLA:HMB2	2.34	0.56
1:A1:431:ASP:OD1	4:D1:46:ALA:N	2.37	0.56
1:A2:204:LEU:HD11	14:A2:1631:CLA:C14	2.36	0.56
1:A4:90:MET:HE3	14:A4:807:CLA:HED2	1.86	0.56
1:A4:352:TRP:CD1	14:A4:824:CLA:H201	2.40	0.56
14:A6:1632:CLA:C3B	14:A6:1633:CLA:HMB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:538:LEU:CD2	14:B1:802:CLA:O2D	2.53	0.56
14:B1:803:CLA:H43	14:B1:833:CLA:HAA2	1.87	0.56
2:B2:318:PHE:HA	14:B2:821:CLA:CAB	2.34	0.56
2:B4:229:TRP:CE3	14:B4:818:CLA:HMB2	2.40	0.56
2:B4:438:GLY:HA3	14:B4:835:CLA:CBB	2.35	0.56
2:B5:360:PRO:HG3	14:B5:1820:CLA:HBA1	1.87	0.56
2:B5:480:LEU:O	2:B5:482:SER:N	2.38	0.56
14:B6:810:CLA:HAA2	10:L6:67:PRO:HG3	1.86	0.56
4:D6:134:LYS:HG2	4:D6:136:TYR:CZ	2.41	0.56
7:I5:20:TRP:NE1	16:I5:102:BCR:HC22	2.20	0.56
14:A3:832:CLA:H12	14:L3:204:CLA:H93	1.86	0.56
1:A5:453:PHE:O	14:L5:203:CLA:CBB	2.54	0.56
1:A5:233:ALA:O	1:A5:235:ASP:N	2.37	0.56
1:A5:440:ILE:HG12	14:A5:831:CLA:CHC	2.36	0.56
1:A6:302:LEU:HD13	14:A6:1615:CLA:HMC1	1.87	0.56
1:A6:544:PHE:CZ	14:B6:802:CLA:HBB1	2.40	0.56
1:A2:651:ARG:NH2	2:B2:643:PRO:HD3	2.20	0.56
2:B5:60:VAL:CG2	14:B5:1830:CLA:H11	2.35	0.56
4:D4:134:LYS:HG2	4:D4:136:TYR:CZ	2.41	0.56
7:I4:20:TRP:CE2	16:I4:102:BCR:HC22	2.41	0.56
9:K1:32:TYR:O	9:K1:34:ILE:N	2.38	0.56
1:A1:691:PHE:CD1	2:B1:670:LEU:HB3	2.41	0.56
1:A6:377:MET:N	1:A6:378:PRO:HD3	2.20	0.56
1:A6:453:PHE:O	14:A6:1633:CLA:CBB	2.53	0.56
2:B1:587:PHE:CB	14:B1:802:CLA:HAC2	2.35	0.56
2:B1:527:HIS:CD2	16:B1:852:BCR:H322	2.41	0.56
1:A6:651:ARG:HB2	2:B6:638:ILE:HG23	1.86	0.56
2:B6:526:HIS:CG	14:B6:838:CLA:HED3	2.41	0.56
8:J4:24:GLY:HA3	14:J4:101:CLA:CBB	2.32	0.56
14:A5:832:CLA:H12	14:L5:205:CLA:H93	1.88	0.56
1:A2:709:ASN:HB3	6:F2:136:ILE:HG23	1.88	0.56
1:A4:352:TRP:HB3	14:A4:804:CLA:HAC1	1.87	0.56
14:A4:838:CLA:H43	14:B4:834:CLA:HAA2	1.88	0.56
1:A4:94:GLY:O	1:A4:98:SER:OG	2.21	0.56
2:B1:304:MET:HG3	2:B1:322:HIS:O	2.06	0.56
2:B1:480:LEU:O	2:B1:482:SER:N	2.38	0.56
2:B1:19:ARG:NH2	2:B1:701:ASP:OD1	2.38	0.56
2:B1:319:ASN:O	17:B1:851:LHG:O5	2.23	0.56
2:B2:497:ASN:O	2:B2:498:VAL:HB	2.05	0.56
2:B4:50:PHE:CD1	2:B4:152:GLY:HA2	2.40	0.56
14:A4:801:CLA:HAB	14:B4:803:CLA:NA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B5:339:TRP:HE1	14:B5:1826:CLA:C1B	2.18	0.56
2:B5:713:LEU:HD23	19:B5:1851:LMG:H122	1.88	0.56
14:B3:1801:CLA:HBA1	14:M3:1601:CLA:HAA2	1.86	0.56
1:A1:285:LEU:HD12	1:A1:518:VAL:HG21	1.87	0.56
1:A1:308:PHE:HE2	14:A1:820:CLA:HAB	1.71	0.56
1:A3:612:HIS:ND1	14:A3:837:CLA:CMC	2.67	0.56
2:B1:438:GLY:HA3	14:B1:834:CLA:CBB	2.35	0.56
2:B1:630:LEU:HD11	14:B1:804:CLA:H93	1.88	0.56
2:B3:525:VAL:HG12	14:B3:1803:CLA:H141	1.87	0.56
2:B4:174:LEU:HG	14:B4:826:CLA:HMD3	1.88	0.56
2:B5:42:TYR:CZ	2:B5:333:LEU:HD21	2.40	0.56
3:C5:52:ARG:O	3:C5:56:ALA:N	2.39	0.56
2:B2:453:GLU:HA	6:F2:48:LEU:HD22	1.88	0.56
6:F3:76:TRP:CH2	14:F3:202:CLA:O1A	2.57	0.56
6:F3:88:VAL:HG11	6:F3:97:LYS:HB2	1.87	0.56
6:F6:73:ILE:O	6:F6:76:TRP:HB3	2.04	0.56
14:B1:841:CLA:H171	7:I1:24:THR:HG23	1.87	0.56
1:A1:79:HIS:CD2	14:A1:804:CLA:HMA1	2.41	0.56
1:A1:372:GLN:HG3	14:A1:825:CLA:CED	2.35	0.56
1:A2:363:MET:HE3	14:A2:1631:CLA:HBC3	1.88	0.56
1:A3:453:PHE:O	14:A3:834:CLA:CBB	2.53	0.56
1:A3:440:ILE:HG12	14:A3:831:CLA:CHC	2.36	0.56
1:A4:577:PRO:O	1:A4:578:CYS:HB3	2.06	0.56
14:A4:840:CLA:H172	8:J4:19:MET:HG3	1.88	0.56
1:A5:259:GLY:O	1:A5:261:PHE:N	2.39	0.56
1:A1:587:CYS:O	2:B1:675:GLY:N	2.39	0.56
2:B3:261:HIS:HD2	2:B3:263:GLN:H	1.54	0.56
2:B3:728:ALA:O	2:B3:732:ILE:HG12	2.05	0.56
2:B4:122:TRP:CZ2	14:B4:815:CLA:H191	2.41	0.56
14:B5:1808:CLA:H143	14:B5:1830:CLA:HBB2	1.88	0.56
2:B6:599:TYR:CE2	14:B6:837:CLA:C2C	2.89	0.56
7:I4:25:VAL:HG21	14:L6:206:CLA:H62	1.88	0.56
8:J3:28:GLU:OE2	14:J3:101:CLA:NA	2.39	0.56
10:L6:68:LEU:HD13	10:L6:73:VAL:HG23	1.88	0.56
12:X4:23:ASN:HD21	14:X4:102:CLA:CHA	2.19	0.56
1:A1:233:ALA:O	1:A1:235:ASP:N	2.37	0.56
1:A2:221:LEU:HB2	1:A2:222:PRO:HD3	1.86	0.56
1:A2:259:GLY:O	1:A2:261:PHE:N	2.39	0.56
1:A2:587:CYS:HB2	2:B2:673:TRP:HB3	1.86	0.56
1:A3:233:ALA:O	1:A3:235:ASP:N	2.37	0.56
2:B1:456:ILE:CD1	14:B1:834:CLA:CHB	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B1:854:CLA:CGA	10:L2:148:ILE:HG23	2.35	0.56
2:B4:660:HIS:CD2	14:B4:801:CLA:O2D	2.58	0.56
2:B5:90:ILE:HG23	14:B5:1811:CLA:O1D	2.04	0.56
2:B5:386:MET:CE	16:B5:1849:BCR:H361	2.36	0.56
2:B5:386:MET:HE1	16:B5:1849:BCR:H363	1.88	0.56
2:B6:50:PHE:CD1	2:B6:152:GLY:HA2	2.41	0.56
14:B6:827:CLA:HBC3	19:B6:848:LMG:H421	1.87	0.56
1:A4:583:ARG:HA	3:C4:75:SER:O	2.05	0.56
10:L3:85:LEU:HD22	10:L3:85:LEU:O	2.06	0.56
1:A4:360:LEU:HD13	14:A4:829:CLA:HBB1	1.87	0.56
1:A6:196:MET:CE	14:A6:1625:CLA:H142	2.36	0.56
2:B1:279:ILE:HD11	14:B1:818:CLA:C4C	2.36	0.56
1:A1:706:TRP:CD1	2:B1:419:GLU:HG3	2.41	0.56
2:B2:390:PHE:HZ	14:B2:824:CLA:HAB	1.71	0.56
2:B2:427:TRP:CE2	14:B2:830:CLA:HBB1	2.41	0.56
2:B4:668:MET:SD	14:B4:805:CLA:NC	2.79	0.56
2:B5:271:ASP:HB3	14:B5:1819:CLA:HMA1	1.88	0.56
14:B6:803:CLA:H43	14:B6:832:CLA:HAA2	1.88	0.56
5:E3:24:ALA:O	5:E3:25:SER:HB3	2.06	0.56
6:F2:69:LEU:HB2	14:F2:204:CLA:HBB2	1.88	0.56
6:F3:76:TRP:NE1	14:F3:202:CLA:HBD	2.21	0.56
14:B2:809:CLA:C4	10:L2:81:SER:HA	2.35	0.56
16:L5:201:BCR:H363	14:L5:204:CLA:CBA	2.35	0.56
14:A1:839:CLA:H171	10:L1:85:LEU:HD11	1.88	0.56
1:A2:377:MET:N	1:A2:378:PRO:HD3	2.21	0.56
14:A5:828:CLA:H93	16:J5:103:BCR:H361	1.88	0.56
2:B1:466:ILE:CG1	14:B1:838:CLA:H43	2.36	0.56
2:B2:140:PHE:CE2	2:B2:144:LEU:HD11	2.40	0.56
2:B4:116:TYR:HA	2:B4:370:THR:HG22	1.86	0.56
2:B4:43:GLN:OE1	2:B4:161:ARG:NH2	2.39	0.56
2:B4:589:MET:HE2	2:B4:590:LEU:HD23	1.87	0.56
14:A4:853:CLA:HAA2	14:B5:1801:CLA:CAA	2.36	0.56
2:B6:275:HIS:HB2	14:B6:817:CLA:CHB	2.36	0.56
2:B2:554:PRO:HD2	3:C2:61:PHE:CZ	2.40	0.56
11:M2:24:ARG:NH2	14:L3:202:CLA:HED2	2.17	0.56
14:A2:1641:CLA:H43	14:B2:831:CLA:HAA2	1.88	0.55
1:A5:207:LEU:HD22	16:A5:846:BCR:H361	1.88	0.55
2:B1:186:SER:HB2	14:B1:819:CLA:HMC3	1.89	0.55
2:B1:279:ILE:CD1	14:B1:818:CLA:HBC3	2.35	0.55
2:B1:346:VAL:HG21	16:B1:847:BCR:H362	1.88	0.55
2:B1:117:SER:HA	14:B1:828:CLA:HMA2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:294:PHE:HE1	14:B3:1814:CLA:HMA1	1.72	0.55
2:B4:480:LEU:O	2:B4:482:SER:N	2.38	0.55
2:B4:376:THR:HG23	2:B4:597:THR:HG21	1.87	0.55
1:A5:564:ARG:O	4:D5:60:ARG:NH1	2.37	0.55
6:F4:65:ILE:HB	6:F4:66:PRO:HD3	1.88	0.55
6:F5:78:GLY:HA3	16:F5:1302:BCR:HC31	1.88	0.55
8:J5:28:GLU:HG3	14:J5:101:CLA:C1B	2.36	0.55
1:A2:387:TYR:CE2	1:A2:622:TRP:CD1	2.95	0.55
16:A4:849:BCR:H403	16:A4:849:BCR:H23C	1.87	0.55
2:B1:500:LEU:O	2:B1:504:LEU:HG	2.06	0.55
2:B1:668:MET:HB2	14:B1:806:CLA:C1C	2.36	0.55
2:B1:693:LEU:HD11	10:L1:34:LEU:HD23	1.88	0.55
2:B3:192:HIS:HE1	14:B3:1816:CLA:C1A	2.19	0.55
2:B5:173:ARG:NH1	14:B5:1815:CLA:HMD2	2.22	0.55
2:B5:425:LEU:HG	14:B5:1841:CLA:CBB	2.36	0.55
3:C2:20:CYS:SG	18:C2:101:SF4:S3	3.04	0.55
6:F6:65:ILE:HB	6:F6:66:PRO:HD3	1.88	0.55
15:B1:842:PQN:H141	14:I1:101:CLA:HBB2	1.87	0.55
12:X2:26:VAL:HB	14:X2:1701:CLA:HED1	1.89	0.55
1:A2:40:ARG:HA	13:P2:60:SER:HB2	1.88	0.55
1:A2:583:ARG:HA	3:C2:76:MET:C	2.26	0.55
1:A2:86:TRP:HA	14:A2:1609:CLA:CBB	2.36	0.55
1:A3:399:TRP:NE1	14:A3:828:CLA:HAB	2.21	0.55
1:A6:356:LEU:O	1:A6:360:LEU:HB2	2.07	0.55
14:B2:826:CLA:HBC3	19:B2:848:LMG:H421	1.89	0.55
2:B6:386:MET:HE1	16:B6:847:BCR:H361	1.89	0.55
3:C2:16:CYS:SG	3:C2:17:VAL:N	2.79	0.55
4:D5:39:PHE:CE1	4:D5:67:LEU:HD11	2.41	0.55
7:I1:30:LEU:HD13	16:I1:103:BCR:HC8	1.86	0.55
8:J6:12:PRO:HA	14:J6:1101:CLA:HED1	1.89	0.55
16:L3:201:BCR:H363	14:L3:203:CLA:CBA	2.36	0.55
10:L3:62:TRP:CE3	10:L3:81:SER:HB2	2.41	0.55
1:A1:207:LEU:HD13	16:A1:843:BCR:H362	1.88	0.55
14:A2:1604:CLA:H2	2:B2:434:PHE:CE2	2.42	0.55
1:A2:352:TRP:HB3	14:A2:1607:CLA:HAC1	1.88	0.55
1:A3:83:VAL:HG11	14:A3:805:CLA:H72	1.89	0.55
1:A4:470:ARG:NH1	2:B4:94:GLN:O	2.38	0.55
1:A5:367:SER:OG	1:A5:397:HIS:O	2.24	0.55
14:A5:839:CLA:H43	14:B5:1834:CLA:HAA2	1.88	0.55
16:A6:1648:BCR:H403	16:A6:1648:BCR:H23C	1.87	0.55
1:A6:587:CYS:O	2:B6:675:GLY:CA	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:185:SER:HB3	14:B1:819:CLA:HBC1	1.89	0.55
14:B3:1829:CLA:HBC3	19:B3:1850:LMG:H421	1.87	0.55
2:B4:360:PRO:HG3	14:B4:820:CLA:CBA	2.36	0.55
2:B5:458:ILE:N	2:B5:458:ILE:HD12	2.22	0.55
14:B2:806:CLA:H102	16:I2:101:BCR:HC31	1.89	0.55
7:I5:21:LEU:O	7:I5:22:MET:C	2.45	0.55
8:J5:27:ILE:HG21	16:J5:104:BCR:H343	1.89	0.55
8:J5:21:ILE:O	14:J5:101:CLA:HBB2	2.06	0.55
10:L4:62:TRP:CE2	14:L4:201:CLA:H12	2.42	0.55
10:L5:139:LEU:HD23	14:L5:206:CLA:H42	1.88	0.55
10:L6:61:PRO:HB3	14:L6:208:CLA:HBB1	1.89	0.55
3:C3:15:GLN:OE1	13:P3:64:PHE:CE2	2.60	0.55
1:A4:40:ARG:HH12	13:P4:63:SER:HB3	1.71	0.55
1:A1:79:HIS:CE1	14:A1:804:CLA:CMA	2.89	0.55
1:A3:120:ILE:O	1:A3:123:GLN:HG2	2.06	0.55
1:A3:651:ARG:NE	1:A3:652:ASP:OD2	2.39	0.55
16:A5:850:BCR:H402	14:B5:1802:CLA:H142	1.88	0.55
2:B1:289:MET:HE1	14:B1:823:CLA:HMD3	1.87	0.55
2:B2:433:GLY:HA2	2:B2:531:LEU:HD22	1.88	0.55
14:B3:1825:CLA:HBB1	14:B3:1832:CLA:HMD2	1.87	0.55
2:B4:696:LEU:HD11	10:L4:36:ALA:HB1	1.88	0.55
2:B5:467:GLN:NE2	14:B5:1839:CLA:OBD	2.35	0.55
14:B5:1842:CLA:HBB2	15:B5:1844:PQN:H141	1.87	0.55
2:B5:122:TRP:CD1	2:B5:361:TYR:CZ	2.95	0.55
2:B5:398:VAL:CG2	2:B5:547:ALA:HB1	2.37	0.55
4:D2:42:PRO:HD3	4:D2:67:LEU:HD13	1.87	0.55
10:L3:79:LEU:HD22	10:L3:136:PHE:CD2	2.41	0.55
11:M4:28:GLU:OE2	11:M4:28:GLU:HA	2.07	0.55
1:A1:436:HIS:NE2	1:A1:440:ILE:HD11	2.22	0.55
1:A3:682:ILE:HD11	16:A3:852:BCR:C15	2.37	0.55
1:A3:300:HIS:HE2	14:A3:819:CLA:C2B	2.18	0.55
1:A4:377:MET:N	1:A4:378:PRO:HD3	2.21	0.55
1:A6:198:ASN:OD1	1:A6:315:TYR:HD1	1.89	0.55
2:B1:318:PHE:CE1	16:B1:846:BCR:H353	2.42	0.55
14:B2:809:CLA:H42	10:L2:81:SER:HA	1.87	0.55
2:B3:434:PHE:CE2	14:B3:1802:CLA:C2	2.90	0.55
1:A4:439:ALA:HA	2:B4:686:TRP:CZ3	2.41	0.55
14:A5:801:CLA:C1A	14:B5:1803:CLA:HAB	2.37	0.55
2:B5:181:LEU:HD13	14:B5:1815:CLA:HBB	1.89	0.55
14:B2:806:CLA:HMD3	7:I2:10:LEU:HD23	1.89	0.55
6:F5:69:LEU:HB2	14:J5:102:CLA:CBB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M1:29:LEU:O	11:M1:30:TYR:HB2	2.07	0.55
11:M3:29:LEU:O	11:M3:30:TYR:HB2	2.07	0.55
1:A1:259:GLY:O	1:A1:261:PHE:N	2.39	0.55
1:A1:58:PHE:CD1	14:A1:804:CLA:HMC2	2.42	0.55
1:A4:455:SER:OG	1:A4:456:PHE:N	2.38	0.55
2:B1:229:TRP:HB2	14:B1:817:CLA:C1	2.29	0.55
2:B1:278:ALA:HB1	14:B1:817:CLA:HBC2	1.89	0.55
14:A3:801:CLA:C1A	14:B3:1803:CLA:HAB	2.37	0.55
14:A3:840:CLA:H43	14:B3:1834:CLA:HAA2	1.89	0.55
2:B3:467:GLN:NE2	14:B3:1839:CLA:OBD	2.40	0.55
16:A4:849:BCR:H402	14:B4:802:CLA:H142	1.88	0.55
2:B4:125:THR:CG2	14:B4:820:CLA:HED1	2.37	0.55
2:B5:622:LEU:HD13	14:B5:1804:CLA:HMA1	1.88	0.55
2:B5:446:VAL:HG13	2:B5:451:THR:O	2.07	0.55
6:F5:65:ILE:HD12	14:J5:102:CLA:HMB3	1.87	0.55
10:L2:77:GLY:O	10:L2:81:SER:OG	2.14	0.55
1:A1:675:LEU:HD11	14:A1:827:CLA:H143	1.88	0.55
1:A1:83:VAL:HG11	14:A1:804:CLA:H72	1.88	0.55
1:A3:259:GLY:O	1:A3:261:PHE:N	2.39	0.55
1:A4:360:LEU:CD1	14:A4:829:CLA:HBB1	2.37	0.55
18:A5:854:SF4:S3	2:B5:574:CYS:SG	3.03	0.55
14:A6:1603:CLA:H142	16:A6:1648:BCR:H402	1.89	0.55
2:B1:59:TRP:NE1	14:B1:828:CLA:OBD	2.33	0.55
14:B1:854:CLA:HBB1	14:B1:854:CLA:HHC	1.88	0.55
2:B3:153:TRP:HZ3	14:B3:1801:CLA:H62	1.71	0.55
2:B3:176:HIS:HB3	14:B3:1815:CLA:CHC	2.37	0.55
2:B5:372:ALA:HB1	2:B5:731:LEU:HD11	1.88	0.55
2:B5:532:GLY:HA2	2:B5:588:TRP:CZ3	2.42	0.55
14:B6:810:CLA:HBB1	14:B6:810:CLA:HHC	1.89	0.55
5:E2:39:ARG:NH2	13:P2:81:TYR:OH	2.37	0.55
1:A1:199:HIS:ND1	14:A1:812:CLA:HMC2	2.22	0.55
1:A3:706:TRP:CD1	2:B3:419:GLU:HG3	2.42	0.55
1:A3:79:HIS:NE2	14:A3:805:CLA:HMA1	2.22	0.55
1:A3:300:HIS:HE2	14:A3:819:CLA:C1B	2.20	0.55
1:A6:352:TRP:CE2	14:A6:1625:CLA:H18	2.42	0.55
2:B1:173:ARG:HG2	14:B1:825:CLA:OBD	2.07	0.55
2:B1:279:ILE:HD13	14:B1:818:CLA:HBC2	1.87	0.55
2:B2:229:TRP:HB2	14:B2:815:CLA:C1	2.22	0.55
2:B2:716:LEU:O	2:B2:720:SER:OG	2.24	0.55
2:B3:116:TYR:HA	2:B3:370:THR:HG22	1.88	0.55
2:B4:300:ILE:HD13	14:B4:826:CLA:CAC	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:21:TRP:CZ2	14:B4:842:CLA:HMB1	2.42	0.55
2:B5:340:HIS:HD2	14:B5:1807:CLA:OBD	1.90	0.55
2:B5:642:ASN:HB2	2:B5:643:PRO:CD	2.37	0.55
5:E6:59:ASN:OD1	5:E6:59:ASN:N	2.39	0.55
6:F2:70:PHE:CD1	16:F2:201:BCR:H321	2.42	0.55
10:L6:129:MET:SD	16:L5:201:BCR:H371	2.47	0.55
3:C3:13:CYS:HB3	13:P3:39:SER:OG	2.06	0.55
1:A5:587:CYS:HB2	2:B5:673:TRP:HB2	1.88	0.55
1:A6:360:LEU:HD11	14:A6:1630:CLA:HBB1	1.88	0.55
2:B1:61:SER:OG	2:B1:138:ALA:O	2.25	0.55
2:B1:53:LEU:HD11	14:B1:807:CLA:CGA	2.35	0.55
2:B2:52:HIS:NE2	14:B2:804:CLA:HMA1	2.22	0.55
1:A3:121:VAL:HB	14:B3:1835:CLA:HMD1	1.89	0.55
2:B3:642:ASN:HB2	2:B3:643:PRO:CD	2.37	0.55
2:B4:282:LEU:HD12	14:B4:821:CLA:HMC1	1.89	0.55
14:B4:842:CLA:HBB2	15:B4:844:PQN:H141	1.89	0.55
14:A4:853:CLA:HAA2	14:B5:1801:CLA:HAA2	1.89	0.55
2:B6:212:LEU:HD21	16:B6:845:BCR:H341	1.89	0.55
3:C5:28:VAL:HG12	4:D5:109:ARG:HB3	1.89	0.55
14:A6:1640:CLA:H172	8:J6:19:MET:HG3	1.89	0.55
14:A3:843:CLA:C15	10:L3:85:LEU:HD21	2.37	0.55
1:A1:352:TRP:CZ3	14:A1:824:CLA:H112	2.41	0.54
1:A2:694:ARG:HD3	2:B2:572:GLY:HA3	1.89	0.54
1:A4:308:PHE:HE2	14:A4:820:CLA:HAB	1.71	0.54
1:A5:443:HIS:CD2	14:A5:831:CLA:HMB1	2.42	0.54
2:B1:122:TRP:CZ2	14:B1:814:CLA:C20	2.80	0.54
2:B1:233:ALA:O	2:B1:234:GLN:O	2.25	0.54
2:B1:45:ILE:HD12	14:B1:807:CLA:C1C	2.37	0.54
2:B1:447:VAL:HG11	2:B1:621:TYR:CE1	2.42	0.54
2:B2:398:VAL:CG2	2:B2:547:ALA:HB1	2.37	0.54
2:B2:724:ILE:HG23	14:B2:826:CLA:CBB	2.36	0.54
14:B2:827:CLA:H51	16:B2:844:BCR:H392	1.89	0.54
2:B2:288:HIS:CE1	16:B2:842:BCR:H363	2.42	0.54
2:B6:304:MET:HG3	2:B6:322:HIS:O	2.07	0.54
3:C2:10:CYS:SG	18:C2:102:SF4:S3	2.99	0.54
9:K4:73:VAL:CA	14:K4:1401:CLA:HBB1	2.33	0.54
1:A1:36:ARG:HH12	13:P1:70:ILE:CB	2.14	0.54
1:A2:440:ILE:HG12	14:A2:1633:CLA:CHC	2.36	0.54
1:A4:440:ILE:HG12	14:A4:830:CLA:CHC	2.37	0.54
2:B1:446:VAL:HG13	2:B1:451:THR:O	2.07	0.54
2:B2:622:LEU:HD11	14:B2:801:CLA:H202	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B2:839:CLA:HBB2	15:B2:841:PQN:H141	1.89	0.54
14:B3:1812:CLA:HHC	14:B3:1812:CLA:HBB1	1.90	0.54
2:B3:347:ILE:CG2	14:B3:1826:CLA:H43	2.37	0.54
14:B4:843:CLA:H171	7:I4:24:THR:HG23	1.89	0.54
14:B6:840:CLA:HBB2	15:B6:842:PQN:H141	1.88	0.54
6:F3:95:ASN:H	6:F3:95:ASN:HD22	1.56	0.54
10:L1:41:LEU:HD21	10:L3:98:LEU:HD21	1.88	0.54
10:L4:117:TRP:O	10:L4:121:THR:OG1	2.20	0.54
10:L4:79:LEU:HD22	10:L4:136:PHE:CD2	2.42	0.54
1:A2:399:TRP:NE1	14:A2:1630:CLA:HAB	2.22	0.54
1:A4:215:HIS:HB2	14:A4:813:CLA:C1C	2.38	0.54
1:A6:691:PHE:HB2	14:A6:1603:CLA:HBC2	1.89	0.54
1:A1:589:VAL:HG13	2:B1:675:GLY:HA3	1.88	0.54
2:B2:642:ASN:HB2	2:B2:643:PRO:CD	2.37	0.54
14:B2:809:CLA:HBB1	14:B2:809:CLA:HHC	1.90	0.54
2:B3:598:PHE:CE1	14:B3:1803:CLA:HED2	2.42	0.54
2:B4:514:LEU:HD12	14:B4:828:CLA:CMC	2.37	0.54
2:B5:261:HIS:CD2	2:B5:263:GLN:H	2.24	0.54
2:B5:541:VAL:O	2:B5:545:LEU:HG	2.08	0.54
6:F6:103:VAL:HB	6:F6:104:PRO:HD3	1.89	0.54
10:L5:89:ALA:HB1	16:L5:207:BCR:H401	1.88	0.54
1:A1:270:PHE:CD1	14:A1:840:CLA:HMD2	2.42	0.54
1:A1:587:CYS:HB2	2:B1:673:TRP:HB3	1.88	0.54
1:A2:189:TRP:CZ2	14:A2:1615:CLA:CAC	2.89	0.54
1:A6:90:MET:HE3	14:A6:1608:CLA:HED2	1.89	0.54
14:A1:801:CLA:C1A	14:B1:804:CLA:HAB	2.38	0.54
2:B2:304:MET:HG3	2:B2:322:HIS:O	2.06	0.54
2:B2:42:TYR:CZ	2:B2:333:LEU:HD21	2.42	0.54
2:B3:373:ALA:HB1	14:B3:1829:CLA:HMA1	1.89	0.54
2:B4:446:VAL:HG13	2:B4:451:THR:O	2.07	0.54
2:B5:233:ALA:O	2:B5:234:GLN:O	2.26	0.54
14:B6:810:CLA:H11	10:L5:148:ILE:HD13	1.88	0.54
8:J2:27:ILE:CG2	16:J2:103:BCR:H343	2.38	0.54
10:L5:92:CYS:HB3	16:L5:207:BCR:C19	2.37	0.54
10:L6:31:ILE:HD13	10:L6:34:LEU:HD22	1.88	0.54
1:A4:744:TRP:HB2	14:A4:827:CLA:HBB1	1.90	0.54
1:A5:470:ARG:NH1	2:B5:94:GLN:O	2.40	0.54
2:B1:272:MET:SD	14:B1:819:CLA:HMA2	2.48	0.54
14:L1:207:CLA:H91	14:B3:1812:CLA:H101	1.88	0.54
2:B3:281:VAL:HG22	16:B3:1845:BCR:H353	1.90	0.54
2:B3:382:ALA:O	2:B3:386:MET:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:651:ARG:NH2	2:B3:643:PRO:HD3	2.22	0.54
2:B4:535:THR:HG23	14:B4:802:CLA:HBD	1.89	0.54
6:F1:78:GLY:HA3	16:F1:1302:BCR:HC31	1.88	0.54
8:J5:24:GLY:HA3	14:J5:101:CLA:CBB	2.34	0.54
1:A2:587:CYS:O	2:B2:675:GLY:CA	2.56	0.54
1:A4:547:HIS:CE1	14:A4:837:CLA:NA	2.75	0.54
1:A6:399:TRP:CD1	14:A6:1628:CLA:HAB	2.42	0.54
2:B2:60:VAL:HG21	14:B2:827:CLA:H42	1.90	0.54
14:B2:832:CLA:H122	6:F2:69:LEU:HD11	1.90	0.54
2:B3:188:ALA:CB	14:B3:1830:CLA:H202	2.38	0.54
2:B3:414:VAL:HA	2:B3:417:HIS:CE1	2.42	0.54
2:B3:45:ILE:HD12	14:B3:1807:CLA:C2C	2.38	0.54
2:B3:531:LEU:HD11	14:B3:1802:CLA:O1A	2.07	0.54
14:B4:812:CLA:HBB1	14:B4:812:CLA:HHC	1.90	0.54
14:B4:852:CLA:H61	14:B4:852:CLA:HBD	1.89	0.54
2:B5:24:ILE:HA	14:B5:1806:CLA:HMD3	1.89	0.54
2:B6:375:TYR:CE2	2:B6:600:TRP:CD1	2.95	0.54
5:E4:37:ILE:HD13	13:P4:41:ARG:HD2	1.86	0.54
14:B3:1806:CLA:C2	11:M3:26:SER:HB2	2.37	0.54
12:X4:23:ASN:HD21	14:X4:102:CLA:C4D	2.21	0.54
1:A1:313:HIS:NE2	16:A1:842:BCR:H363	2.22	0.54
1:A2:587:CYS:O	2:B2:675:GLY:HA3	2.08	0.54
1:A3:297:THR:O	1:A3:300:HIS:HB3	2.07	0.54
2:B1:211:PHE:HB3	14:B1:815:CLA:HMD3	1.89	0.54
2:B1:493:PRO:HG3	14:B1:837:CLA:CHD	2.37	0.54
2:B2:630:LEU:CD1	14:B2:801:CLA:H93	2.38	0.54
2:B3:256:PHE:CE1	14:B3:1819:CLA:CAB	2.87	0.54
2:B4:141:LEU:HD23	2:B4:144:LEU:HD12	1.88	0.54
1:A5:655:TRP:CD1	2:B5:631:TRP:CD1	2.96	0.54
14:B6:810:CLA:H42	10:L6:81:SER:HA	1.90	0.54
1:A4:564:ARG:HB3	3:C4:79:ALA:HB3	1.90	0.54
3:C6:33:CYS:SG	3:C6:34:LYS:N	2.80	0.54
4:D4:39:PHE:CE1	4:D4:67:LEU:HD11	2.43	0.54
5:E3:3:ARG:HH12	13:P3:31:GLU:CB	2.08	0.54
7:I1:21:LEU:O	7:I1:25:VAL:HG23	2.08	0.54
1:A1:204:LEU:HD11	14:A1:828:CLA:H141	1.89	0.54
1:A3:444:LEU:HB2	14:A3:839:CLA:CBB	2.37	0.54
1:A5:313:HIS:CE1	16:A5:845:BCR:C36	2.82	0.54
11:M4:21:LEU:HD21	14:A6:1601:CLA:HMA1	1.90	0.54
2:B1:1:ALA:O	7:I1:38:ALA:N	2.41	0.54
2:B3:599:TYR:HD2	14:B3:1839:CLA:HMC2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B3:1842:CLA:HBB2	15:B3:1844:PQN:H141	1.89	0.54
14:B4:830:CLA:H51	16:B4:847:BCR:H392	1.89	0.54
2:B5:50:PHE:CD1	2:B5:152:GLY:HA2	2.42	0.54
2:B6:7:PHE:CD1	2:B6:33:HIS:CD2	2.95	0.54
5:E2:15:TYR:CE2	5:E2:44:ASN:HA	2.42	0.54
9:K3:73:VAL:HA	14:K3:1401:CLA:HBB1	1.90	0.54
10:L6:145:VAL:HA	10:L6:148:ILE:HD12	1.90	0.54
7:I4:29:LEU:CD2	14:L6:206:CLA:HBC3	2.38	0.54
16:A3:852:BCR:H402	14:B3:1802:CLA:H142	1.89	0.54
14:A5:808:CLA:H112	14:A5:830:CLA:H203	1.90	0.54
1:A6:50:ASN:OD1	17:A6:1649:LHG:HC11	2.07	0.54
2:B1:289:MET:CE	14:B1:823:CLA:HMD3	2.38	0.54
2:B1:398:VAL:CG2	2:B1:547:ALA:HB1	2.38	0.54
2:B3:188:ALA:HA	14:B3:1817:CLA:CBB	2.38	0.54
2:B3:688:HIS:HE1	2:B3:697:VAL:O	1.90	0.54
2:B4:479:THR:O	2:B4:480:LEU:O	2.26	0.54
2:B4:693:LEU:HD12	14:L4:204:CLA:H11	1.89	0.54
2:B6:278:ALA:HB2	14:B6:817:CLA:CBB	2.35	0.54
2:B6:479:THR:O	2:B6:480:LEU:O	2.26	0.54
5:E2:3:ARG:HH12	13:P2:31:GLU:HB2	1.72	0.54
6:F1:103:VAL:HB	6:F1:104:PRO:HD3	1.90	0.54
6:F6:88:VAL:HG11	6:F6:97:LYS:HB2	1.90	0.54
10:L1:79:LEU:HD22	10:L1:136:PHE:CG	2.43	0.54
10:L3:57:PHE:HB2	14:L3:205:CLA:C4C	2.38	0.54
1:A1:269:THR:O	1:A1:270:PHE:HB2	2.08	0.54
1:A2:468:PHE:CZ	14:B2:808:CLA:CHC	2.91	0.54
1:A4:221:LEU:HD11	1:A4:295:SER:HA	1.89	0.54
1:A4:50:ASN:OD1	17:A4:850:LHG:HC11	2.07	0.54
1:A5:590:SER:OG	1:A5:593:ASP:OD2	2.24	0.54
1:A6:84:PHE:CE1	14:A6:1605:CLA:H91	2.42	0.54
2:B1:654:TRP:CZ2	14:B1:801:CLA:H72	2.43	0.54
2:B2:390:PHE:CZ	14:B2:824:CLA:HAB	2.43	0.54
14:B3:1801:CLA:H61	14:B3:1801:CLA:HBD	1.90	0.54
2:B3:662:VAL:HG22	14:B3:1843:CLA:HMB3	1.88	0.54
2:B4:59:TRP:HB2	14:B4:810:CLA:H192	1.90	0.54
2:B5:150:PHE:CZ	14:B5:1801:CLA:H2	2.43	0.54
2:B5:433:GLY:HA2	2:B5:531:LEU:HD22	1.89	0.54
2:B5:61:SER:OG	2:B5:138:ALA:O	2.26	0.54
2:B6:233:ALA:O	2:B6:234:GLN:O	2.26	0.54
14:B6:832:CLA:CBB	14:B6:833:CLA:HMB2	2.38	0.54
7:I4:20:TRP:CD2	16:I4:102:BCR:HC31	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J5:31:ARG:CD	16:J5:104:BCR:H312	2.26	0.54
8:J5:27:ILE:HG21	16:J5:104:BCR:C34	2.37	0.54
10:L6:46:ARG:O	10:L6:50:VAL:HG23	2.07	0.54
1:A1:377:MET:N	1:A1:378:PRO:HD3	2.24	0.53
1:A1:484:PRO:HB3	14:A1:835:CLA:HED3	1.90	0.53
14:A2:1610:CLA:H112	14:A2:1632:CLA:H203	1.90	0.53
1:A6:259:GLY:C	1:A6:261:PHE:H	2.12	0.53
1:A6:280:THR:OG1	1:A6:296:ASP:OD1	2.17	0.53
1:A6:385:THR:HG23	1:A6:523:LYS:HB2	1.90	0.53
2:B1:431:PHE:HA	14:B1:833:CLA:O1D	2.07	0.53
2:B1:494:ASN:HB3	14:B1:837:CLA:O1D	2.08	0.53
14:B1:829:CLA:H51	16:B1:845:BCR:H392	1.89	0.53
2:B3:181:LEU:HD21	14:B3:1815:CLA:H12	1.90	0.53
2:B4:340:HIS:HD2	14:B4:807:CLA:OBD	1.90	0.53
2:B5:625:TRP:HB3	14:B5:1803:CLA:H91	1.90	0.53
2:B6:289:MET:HG3	14:B6:821:CLA:C4C	2.38	0.53
3:C3:16:CYS:SG	3:C3:17:VAL:N	2.81	0.53
1:A4:583:ARG:HA	3:C4:76:MET:HA	1.90	0.53
5:E6:3:ARG:HH12	13:P6:31:GLU:HB2	1.74	0.53
1:A2:194:GLU:HG2	1:A2:315:TYR:HB3	1.90	0.53
1:A2:308:PHE:HE2	14:A2:1623:CLA:HAB	1.73	0.53
1:A3:377:MET:N	1:A3:378:PRO:HD3	2.23	0.53
1:A3:396:HIS:HE2	14:A3:829:CLA:C1B	2.21	0.53
1:A3:387:TYR:CE2	1:A3:622:TRP:CD1	2.96	0.53
2:B1:430:LEU:HD11	16:B1:848:BCR:H403	1.90	0.53
2:B1:319:ASN:ND2	17:B1:851:LHG:O4	2.39	0.53
2:B2:532:GLY:HA2	2:B2:588:TRP:CZ3	2.43	0.53
2:B4:174:LEU:HD11	14:B4:826:CLA:CHD	2.38	0.53
2:B4:458:ILE:HD12	2:B4:458:ILE:N	2.23	0.53
2:B5:339:TRP:HZ2	14:B5:1826:CLA:CAB	2.19	0.53
2:B5:625:TRP:CH2	14:B5:1803:CLA:H142	2.43	0.53
3:C3:14:THR:HG22	3:C3:27:MET:HG3	1.90	0.53
6:F1:69:LEU:HB2	14:J1:102:CLA:HBB1	1.91	0.53
9:K4:40:GLY:O	9:K4:41:PRO:C	2.45	0.53
1:A2:681:PHE:CD2	16:A2:1652:BCR:H363	2.43	0.53
1:A3:231:VAL:O	1:A3:232:ALA:CB	2.57	0.53
1:A4:86:TRP:HE1	14:A4:807:CLA:HBA1	1.74	0.53
1:A5:204:LEU:HD11	14:A5:829:CLA:H141	1.89	0.53
1:A5:675:LEU:HD11	14:A5:828:CLA:H143	1.90	0.53
14:A6:1608:CLA:H112	14:A6:1630:CLA:H203	1.90	0.53
2:B1:642:ASN:HB2	2:B1:643:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:587:CYS:HB2	2:B1:673:TRP:CB	2.38	0.53
16:A1:847:BCR:H402	14:B1:802:CLA:H142	1.89	0.53
2:B3:599:TYR:CZ	14:B3:1839:CLA:HBC2	2.44	0.53
14:B3:1831:CLA:H143	19:B3:1850:LMG:H231	1.90	0.53
2:B5:157:GLN:O	2:B5:161:ARG:HG3	2.07	0.53
2:B5:173:ARG:HH11	14:B5:1815:CLA:HMD2	1.73	0.53
2:B6:70:GLN:OE1	2:B6:88:HIS:HB2	2.08	0.53
14:A3:834:CLA:H12	10:L3:62:TRP:CE2	2.43	0.53
1:A1:445:ASN:HD22	2:B1:680:LEU:HD11	1.73	0.53
14:A2:1604:CLA:H142	16:A2:1652:BCR:H402	1.90	0.53
1:A3:353:HIS:CD2	14:A3:805:CLA:HBC1	2.44	0.53
1:A6:683:TRP:CE2	14:A6:1602:CLA:HBA2	2.43	0.53
2:B1:402:ASP:O	2:B1:406:ASN:OD1	2.26	0.53
2:B1:45:ILE:CD1	14:B1:807:CLA:HMC2	2.38	0.53
2:B2:479:THR:O	2:B2:480:LEU:O	2.26	0.53
2:B4:52:HIS:CE1	14:B4:807:CLA:CMA	2.91	0.53
1:A5:121:VAL:HB	14:B5:1835:CLA:HMD1	1.89	0.53
2:B5:304:MET:HG3	2:B5:322:HIS:O	2.08	0.53
2:B5:625:TRP:CB	14:B5:1803:CLA:H91	2.38	0.53
2:B6:493:PRO:HG3	14:B6:836:CLA:C1D	2.38	0.53
3:C3:28:VAL:HG12	4:D3:109:ARG:HB3	1.89	0.53
4:D4:60:ARG:N	4:D4:63:GLN:OE1	2.42	0.53
1:A1:601:TRP:HH2	14:B1:801:CLA:HBB1	1.73	0.53
2:B1:179:ALA:HB2	2:B1:287:GLY:HA3	1.91	0.53
2:B1:208:TRP:CD1	14:B1:815:CLA:CAD	2.92	0.53
1:A1:439:ALA:HA	2:B1:686:TRP:CZ3	2.44	0.53
2:B3:48:SER:HG	14:B3:1807:CLA:HBB1	1.69	0.53
2:B4:532:GLY:HA2	2:B4:588:TRP:HZ3	1.73	0.53
2:B4:680:LEU:O	2:B4:684:LEU:HG	2.09	0.53
2:B6:25:ALA:HA	14:B6:829:CLA:H42	1.91	0.53
8:J5:12:PRO:HB2	16:J5:104:BCR:H391	1.91	0.53
10:L2:62:TRP:HZ2	16:L2:203:BCR:C34	2.21	0.53
11:M6:31:LYS:OXT	14:M6:1201:CLA:O1D	2.27	0.53
1:A1:612:HIS:ND1	14:A1:834:CLA:HMC2	2.24	0.53
1:A1:71:LYS:HZ3	14:A1:810:CLA:HED2	1.72	0.53
1:A1:272:TRP:CD1	14:A1:816:CLA:HMB2	2.43	0.53
1:A3:741:ALA:HB2	16:A3:852:BCR:H323	1.91	0.53
1:A3:660:GLN:HG2	1:A3:753:SER:HB3	1.91	0.53
1:A4:681:PHE:CG	16:A4:849:BCR:H363	2.43	0.53
1:A6:196:MET:HE1	14:A6:1625:CLA:H142	1.89	0.53
1:A6:231:VAL:O	1:A6:232:ALA:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:275:HIS:HE1	14:B1:818:CLA:C1D	2.21	0.53
2:B1:442:HIS:CE1	14:B1:834:CLA:C4D	2.90	0.53
2:B1:539:ILE:HG12	14:B1:802:CLA:CMD	2.39	0.53
2:B1:738:LYS:O	2:B1:739:PHE:CB	2.57	0.53
14:B1:854:CLA:H203	14:L2:207:CLA:HMD1	1.91	0.53
2:B3:479:THR:O	2:B3:480:LEU:O	2.27	0.53
2:B3:537:THR:HG21	14:B3:1827:CLA:CBB	2.39	0.53
2:B5:664:ALA:HB3	14:B5:1805:CLA:CBB	2.38	0.53
3:C6:65:ARG:HG2	3:C6:67:TYR:CZ	2.44	0.53
4:D1:10:TYR:HH	4:D1:13:SER:HG	1.55	0.53
4:D3:43:THR:O	4:D3:44:ALA:HB3	2.09	0.53
10:L5:52:MET:HE2	14:L5:204:CLA:H2A	1.90	0.53
1:A3:189:TRP:CZ2	14:A3:810:CLA:HMA1	2.43	0.53
14:A4:801:CLA:C1A	14:B4:803:CLA:HAB	2.39	0.53
14:A6:1602:CLA:C1A	14:B6:804:CLA:HAB	2.38	0.53
2:B1:150:PHE:HZ	14:B1:853:CLA:H2	1.72	0.53
2:B1:227:GLY:O	14:B1:817:CLA:H42	2.09	0.53
2:B1:230:GLY:CA	14:B1:817:CLA:CBA	2.87	0.53
2:B2:458:ILE:N	2:B2:458:ILE:HD12	2.24	0.53
14:B2:831:CLA:CBB	14:B2:832:CLA:HMB2	2.39	0.53
2:B3:503:TRP:CE3	14:B3:1819:CLA:H11	2.43	0.53
2:B4:189:TRP:CZ3	2:B4:192:HIS:CD2	2.96	0.53
2:B5:179:ALA:HB2	2:B5:287:GLY:HA3	1.91	0.53
14:B5:1801:CLA:HBD	14:B5:1801:CLA:H61	1.90	0.53
2:B5:463:ALA:HB2	14:B5:1840:CLA:O2D	2.09	0.53
9:K3:40:GLY:O	9:K3:41:PRO:C	2.46	0.53
9:K6:40:GLY:O	9:K6:41:PRO:C	2.47	0.53
10:L1:58:LEU:HD13	10:L1:85:LEU:HD12	1.91	0.53
14:B6:810:CLA:H91	14:L5:206:CLA:H93	1.91	0.53
12:X3:9:TYR:HA	17:X3:101:LHG:O1	2.08	0.53
1:A3:603:TYR:OH	14:A3:801:CLA:HBA1	2.09	0.53
1:A4:28:TRP:CZ2	14:A4:803:CLA:H11	2.44	0.53
14:A5:843:CLA:H61	14:A5:843:CLA:HBD	1.91	0.53
1:A6:484:PRO:HB3	14:A6:1637:CLA:HED3	1.90	0.53
2:B1:592:THR:O	2:B1:596:VAL:HG13	2.09	0.53
2:B4:233:ALA:O	2:B4:234:GLN:O	2.25	0.53
2:B4:593:ILE:O	2:B4:597:THR:HG23	2.09	0.53
2:B5:140:PHE:CE2	2:B5:144:LEU:HD11	2.43	0.53
2:B6:261:HIS:HD2	2:B6:263:GLN:H	1.57	0.53
2:B6:318:PHE:CD1	14:B6:822:CLA:HAB	2.44	0.53
3:C5:80:TYR:HB3	4:D5:18:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:37:GLN:NE2	4:D1:105:VAL:HG22	2.24	0.53
5:E2:39:ARG:CZ	13:P2:24:TYR:CE2	2.92	0.53
8:J2:21:ILE:HA	14:J2:101:CLA:HBB2	1.91	0.53
10:L6:62:TRP:HZ2	16:L6:204:BCR:C9	2.22	0.53
1:A1:90:MET:HE2	14:A1:827:CLA:HED1	1.91	0.53
1:A3:280:THR:OG1	1:A3:296:ASP:OD1	2.19	0.53
1:A5:231:VAL:O	1:A5:232:ALA:CB	2.57	0.53
1:A5:377:MET:N	1:A5:378:PRO:HD3	2.23	0.53
14:B1:808:CLA:H102	14:B1:808:CLA:H151	1.90	0.53
2:B2:233:ALA:O	2:B2:234:GLN:O	2.26	0.53
2:B2:428:VAL:HG12	2:B2:432:LEU:HD12	1.91	0.53
2:B3:433:GLY:HA2	2:B3:531:LEU:HD22	1.91	0.53
14:B4:812:CLA:H61	7:I4:20:TRP:CZ3	2.44	0.53
2:B5:525:VAL:CG1	14:B5:1803:CLA:H141	2.35	0.53
2:B5:187:LEU:HD11	16:B5:1845:BCR:H342	1.91	0.53
2:B5:514:LEU:CD1	14:B5:1828:CLA:CMC	2.87	0.53
4:D5:43:THR:O	4:D5:44:ALA:HB3	2.09	0.53
6:F5:103:VAL:HG12	6:F5:107:ILE:HD11	1.91	0.53
6:F6:76:TRP:CH2	14:F6:202:CLA:CGA	2.92	0.53
14:A6:1628:CLA:H93	16:J6:1104:BCR:H20C	1.91	0.53
10:L2:135:ALA:O	10:L2:139:LEU:HG	2.08	0.53
10:L5:116:GLY:O	10:L5:117:TRP:C	2.45	0.53
14:B5:1809:CLA:H41	11:M5:12:LEU:HD21	1.90	0.53
1:A1:221:LEU:HB2	1:A1:222:PRO:HD3	1.90	0.53
14:A1:807:CLA:H112	14:A1:829:CLA:H203	1.91	0.53
14:A2:1602:CLA:C1A	14:B2:801:CLA:HAB	2.39	0.53
1:A2:189:TRP:CZ3	14:A2:1615:CLA:HMD3	2.44	0.53
2:B2:174:LEU:HD21	14:B2:823:CLA:C1D	2.39	0.53
2:B2:504:LEU:O	2:B2:508:ASN:ND2	2.42	0.53
2:B2:122:TRP:HZ2	14:B2:812:CLA:H191	1.74	0.53
14:L1:207:CLA:C9	14:B3:1812:CLA:H91	2.35	0.53
14:B3:1830:CLA:H51	16:B3:1847:BCR:H392	1.90	0.53
2:B3:233:ALA:O	2:B3:234:GLN:O	2.26	0.53
2:B4:179:ALA:HB2	2:B4:287:GLY:HA3	1.91	0.53
2:B5:479:THR:O	2:B5:480:LEU:O	2.26	0.53
2:B5:601:HIS:HB3	2:B5:629:TYR:OH	2.08	0.53
4:D1:56:VAL:HA	10:L1:13:PHE:CZ	2.44	0.53
6:F2:73:ILE:O	6:F2:76:TRP:HB3	2.09	0.53
8:J3:33:TYR:N	8:J3:34:PRO:HD3	2.24	0.53
10:L5:106:SER:OG	10:L5:107:SER:N	2.41	0.53
11:M4:13:VAL:HG23	16:M4:101:BCR:H402	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:604:ASN:ND2	14:A1:801:CLA:H201	2.23	0.52
1:A2:56:HIS:HA	1:A2:58:PHE:CE2	2.45	0.52
1:A3:323:HIS:HB3	1:A3:328:ILE:HD11	1.91	0.52
1:A4:548:VAL:HB	1:A4:601:TRP:CZ3	2.44	0.52
1:A4:180:TYR:CE2	14:A4:810:CLA:C4D	2.92	0.52
1:A5:391:LEU:O	1:A5:395:THR:HG23	2.10	0.52
1:A5:86:TRP:O	1:A5:90:MET:HG2	2.09	0.52
11:M4:24:ARG:NH2	14:A6:1601:CLA:HED2	2.22	0.52
1:A6:189:TRP:CZ2	14:A6:1613:CLA:HAC2	2.44	0.52
2:B1:335:PHE:CE1	16:B1:847:BCR:H292	2.44	0.52
2:B1:430:LEU:HD11	16:B1:848:BCR:H402	1.91	0.52
2:B1:496:GLY:HA3	14:B1:836:CLA:HED2	1.91	0.52
2:B2:390:PHE:CD1	2:B2:540:LEU:HD13	2.44	0.52
2:B2:630:LEU:HD12	14:B2:801:CLA:H93	1.92	0.52
14:B2:828:CLA:H143	19:B2:848:LMG:H231	1.91	0.52
2:B4:431:PHE:CZ	16:F4:204:BCR:HC41	2.44	0.52
14:B4:831:CLA:H143	19:B4:851:LMG:H231	1.91	0.52
14:B5:1834:CLA:CBB	14:B5:1835:CLA:HMB2	2.39	0.52
2:B5:386:MET:CE	16:B5:1849:BCR:C36	2.86	0.52
14:B6:829:CLA:H143	19:B6:848:LMG:H231	1.91	0.52
7:I5:10:LEU:N	7:I5:11:PRO:CD	2.71	0.52
11:M5:29:LEU:O	11:M5:30:TYR:HB2	2.09	0.52
1:A1:237:PRO:HB2	1:A1:242:PHE:CE1	2.44	0.52
14:A2:1603:CLA:OBD	14:B2:801:CLA:HMB3	2.10	0.52
1:A2:391:LEU:O	1:A2:395:THR:HG23	2.09	0.52
14:A3:806:CLA:H3A	14:A3:830:CLA:HAB	1.92	0.52
14:A4:807:CLA:H112	14:A4:829:CLA:H203	1.91	0.52
1:A5:403:PHE:HB3	14:A5:806:CLA:H112	1.90	0.52
1:A6:502:ALA:N	1:A6:503:PRO:HD3	2.24	0.52
2:B1:294:PHE:CE1	14:B1:821:CLA:HBD	2.44	0.52
2:B1:466:ILE:HD12	14:B1:838:CLA:O2A	2.09	0.52
2:B4:457:LEU:HD12	6:F4:49:PRO:O	2.09	0.52
2:B5:481:LEU:CD1	14:B5:1836:CLA:HED3	2.38	0.52
2:B5:92:ASP:HB3	2:B5:95:PHE:CE2	2.44	0.52
2:B6:738:LYS:O	2:B6:739:PHE:CB	2.57	0.52
3:C4:24:VAL:O	3:C4:42:PRO:HD2	2.09	0.52
10:L4:48:LEU:HD11	10:L5:125:PHE:CD2	2.44	0.52
1:A3:481:GLN:OE1	1:A3:483:GLN:NE2	2.42	0.52
14:A5:830:CLA:H111	17:A5:851:LHG:H202	1.91	0.52
2:B1:386:MET:HG3	14:B1:826:CLA:C4C	2.39	0.52
14:B1:853:CLA:HBD	14:B1:853:CLA:H61	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:344:LEU:O	2:B2:348:THR:OG1	2.25	0.52
2:B2:256:PHE:CE1	14:B2:816:CLA:HAB	2.44	0.52
2:B2:350:LEU:N	14:B2:824:CLA:HED3	2.25	0.52
2:B3:347:ILE:HG21	14:B3:1826:CLA:H43	1.92	0.52
14:B5:1812:CLA:HBB1	14:B5:1812:CLA:HHC	1.90	0.52
2:B5:532:GLY:HA3	2:B5:592:THR:HG23	1.90	0.52
2:B5:532:GLY:HA2	2:B5:588:TRP:HZ3	1.74	0.52
2:B6:497:ASN:O	2:B6:498:VAL:HB	2.10	0.52
2:B6:303:MET:HA	14:B6:822:CLA:O1D	2.10	0.52
2:B6:421:ILE:HG12	14:B6:830:CLA:CHC	2.40	0.52
6:F1:52:VAL:HG12	6:F1:54:ASP:HB2	1.92	0.52
6:F2:53:VAL:HG12	6:F2:63:PHE:HB2	1.90	0.52
6:F6:110:MET:HB3	14:F6:202:CLA:HED2	1.90	0.52
7:I3:22:MET:C	7:I3:22:MET:SD	2.88	0.52
14:A1:827:CLA:H93	16:J1:103:BCR:H20C	1.91	0.52
6:F3:34:ARG:HD3	8:J3:35:ASP:CG	2.29	0.52
14:A4:827:CLA:H93	16:J4:103:BCR:H20C	1.91	0.52
14:L6:206:CLA:C1B	14:L6:207:CLA:HED1	2.40	0.52
1:A1:367:SER:OG	1:A1:397:HIS:O	2.27	0.52
16:A1:847:BCR:H362	14:B1:805:CLA:C4	2.36	0.52
14:A3:808:CLA:H112	14:A3:830:CLA:H203	1.91	0.52
14:A3:828:CLA:H93	16:J3:103:BCR:H20C	1.91	0.52
1:A5:300:HIS:HE2	14:A5:819:CLA:C1B	2.22	0.52
2:B1:189:TRP:CZ2	14:B1:819:CLA:CAD	2.92	0.52
2:B1:435:HIS:HA	14:B1:834:CLA:HBB2	1.91	0.52
2:B1:466:ILE:CD1	14:B1:838:CLA:H43	2.39	0.52
2:B1:532:GLY:HA2	2:B1:588:TRP:CZ3	2.44	0.52
2:B3:179:ALA:HB2	2:B3:287:GLY:HA3	1.90	0.52
2:B3:288:HIS:C	14:B3:1822:CLA:HED1	2.30	0.52
2:B3:738:LYS:O	2:B3:739:PHE:CB	2.57	0.52
14:B4:834:CLA:CBB	14:B4:835:CLA:HMB2	2.40	0.52
4:D4:43:THR:O	4:D4:44:ALA:HB3	2.09	0.52
6:F3:73:ILE:O	6:F3:76:TRP:HB3	2.08	0.52
8:J6:16:ALA:HA	14:J6:1101:CLA:H8	1.91	0.52
14:L2:205:CLA:C1B	14:L2:206:CLA:HED1	2.39	0.52
10:L2:38:ARG:O	10:L2:46:ARG:NH2	2.42	0.52
1:A2:691:PHE:HB2	14:A2:1604:CLA:HBC2	1.92	0.52
1:A4:302:LEU:HD13	14:A4:814:CLA:HMC1	1.91	0.52
14:B1:830:CLA:H143	19:B1:850:LMG:H231	1.91	0.52
2:B2:45:ILE:HD12	14:B2:804:CLA:C2C	2.40	0.52
2:B3:166:TRP:CE2	14:B3:1813:CLA:CMA	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:153:TRP:HZ3	14:B4:852:CLA:H62	1.74	0.52
2:B5:122:TRP:HH2	16:B5:1847:BCR:H391	1.74	0.52
6:F2:65:ILE:HB	6:F2:66:PRO:HD3	1.92	0.52
14:B3:1835:CLA:C1	8:J3:29:PHE:CE2	2.93	0.52
9:K6:73:VAL:CA	14:K6:1401:CLA:HBB1	2.25	0.52
11:M4:26:SER:HA	11:M4:29:LEU:HD12	1.90	0.52
1:A1:583:ARG:HA	3:C1:75:SER:O	2.09	0.52
1:A1:275:TYR:CZ	14:A1:814:CLA:HMD2	2.45	0.52
14:A2:1623:CLA:HMB2	14:A2:1627:CLA:HMA3	1.92	0.52
1:A2:453:PHE:CZ	14:B2:803:CLA:H12	2.44	0.52
14:A3:845:CLA:H61	14:A3:845:CLA:HBD	1.90	0.52
1:A4:578:CYS:HG	18:A4:852:SF4:FE3	0.49	0.52
14:A5:805:CLA:H71	16:A5:847:BCR:H402	1.92	0.52
14:A5:827:CLA:HMB3	14:A5:834:CLA:H12	1.92	0.52
1:A6:360:LEU:HD13	14:A6:1630:CLA:HBB1	1.92	0.52
1:A6:701:ILE:HA	1:A6:704:ILE:HD12	1.92	0.52
2:B3:497:ASN:O	2:B3:498:VAL:HB	2.09	0.52
2:B3:592:THR:O	2:B3:596:VAL:HG13	2.09	0.52
2:B3:647:ASN:HD22	2:B3:649:LEU:H	1.58	0.52
14:B5:1830:CLA:H51	16:B5:1847:BCR:H392	1.90	0.52
3:C6:72:THR:N	3:C6:75:SER:OG	2.35	0.52
1:A1:435:ARG:HD2	4:D1:12:GLY:O	2.09	0.52
16:F4:204:BCR:H21C	8:J4:39:HIS:HA	1.92	0.52
2:B5:110:ASN:HB3	7:I5:3:GLY:HA2	1.91	0.52
14:L4:203:CLA:H171	7:I5:24:THR:HG21	1.90	0.52
1:A1:28:TRP:CZ2	14:A1:803:CLA:H11	2.45	0.52
1:A2:100:TYR:CE2	1:A2:104:LEU:HD11	2.45	0.52
14:A2:1630:CLA:H93	16:J2:102:BCR:H20C	1.92	0.52
1:A2:231:VAL:O	1:A2:232:ALA:CB	2.58	0.52
1:A3:314:MET:HG3	14:A3:822:CLA:C4C	2.40	0.52
1:A3:675:LEU:HD11	14:A3:828:CLA:H143	1.92	0.52
1:A4:269:THR:O	1:A4:270:PHE:HB2	2.10	0.52
1:A4:447:VAL:HG21	14:A4:837:CLA:C2C	2.40	0.52
1:A5:210:LEU:HD21	16:A5:845:BCR:H342	1.92	0.52
14:A6:1630:CLA:H111	17:A6:1649:LHG:H202	1.92	0.52
2:B3:494:ASN:OD1	14:B3:1838:CLA:O1D	2.28	0.52
2:B3:425:LEU:HG	14:B3:1841:CLA:HBB1	1.87	0.52
2:B4:340:HIS:CD2	14:B4:807:CLA:OBD	2.63	0.52
2:B5:555:ASP:OD1	2:B5:555:ASP:N	2.40	0.52
2:B6:256:PHE:CE1	14:B6:817:CLA:HAB	2.44	0.52
14:B6:802:CLA:OBD	14:B6:804:CLA:HMB3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B1:811:CLA:H192	7:I1:26:VAL:HG21	1.92	0.52
9:K2:40:GLY:O	9:K2:41:PRO:C	2.47	0.52
5:E2:57:THR:CG2	13:P2:42:ALA:HA	2.40	0.52
1:A1:53:ALA:O	14:A1:829:CLA:O1A	2.28	0.52
14:A1:839:CLA:HMA1	2:B1:694:ALA:CB	2.40	0.52
1:A2:612:HIS:ND1	14:A2:1638:CLA:HMC2	2.25	0.52
1:A2:484:PRO:HB3	14:A2:1639:CLA:HED3	1.91	0.52
1:A2:686:SER:HB3	1:A2:734:HIS:CB	2.39	0.52
1:A5:269:THR:O	1:A5:270:PHE:HB2	2.10	0.52
1:A6:587:CYS:O	2:B6:675:GLY:N	2.43	0.52
2:B2:661:LEU:O	2:B2:665:THR:OG1	2.23	0.52
2:B2:354:HIS:CE1	14:B2:825:CLA:C1B	2.93	0.52
2:B3:467:GLN:NE2	14:B3:1839:CLA:HMD1	2.23	0.52
2:B5:738:LYS:O	2:B5:739:PHE:CB	2.57	0.52
2:B6:398:VAL:CG2	2:B6:547:ALA:HB1	2.40	0.52
2:B6:564:PRO:O	2:B6:565:CYS:HB3	2.10	0.52
6:F2:23:ASN:OD1	6:F2:23:ASN:N	2.43	0.52
7:I5:30:LEU:O	7:I5:31:PHE:C	2.47	0.52
5:E2:39:ARG:CZ	13:P2:24:TYR:CZ	2.93	0.52
1:A1:231:VAL:O	1:A1:232:ALA:CB	2.58	0.52
1:A1:36:ARG:CZ	13:P1:70:ILE:CG2	2.86	0.52
1:A1:336:PHE:CB	17:A1:849:LHG:HC41	2.39	0.52
1:A3:399:TRP:CH2	1:A3:740:ILE:HG12	2.45	0.52
1:A3:215:HIS:HB2	14:A3:814:CLA:C1C	2.40	0.52
1:A5:120:ILE:O	1:A5:123:GLN:HG2	2.10	0.52
1:A5:356:LEU:O	1:A5:360:LEU:HB2	2.09	0.52
14:A6:1606:CLA:H3A	14:A6:1630:CLA:HAB	1.92	0.52
1:A6:257:ASP:OD1	1:A6:258:TRP:N	2.43	0.52
2:B1:497:ASN:O	2:B1:498:VAL:HB	2.10	0.52
2:B2:573:THR:O	2:B2:576:ILE:HB	2.10	0.52
1:A2:587:CYS:CB	2:B2:673:TRP:HB3	2.40	0.52
2:B3:487:ILE:HG12	14:B3:1837:CLA:CMD	2.40	0.52
2:B4:59:TRP:HA	14:B4:809:CLA:CBB	2.39	0.52
2:B4:318:PHE:CE1	16:B4:848:BCR:H353	2.45	0.52
4:D2:43:THR:O	4:D2:44:ALA:HB3	2.10	0.52
14:B1:854:CLA:CMB	7:I1:20:TRP:CZ2	2.82	0.52
10:L2:62:TRP:HZ2	16:L2:203:BCR:H342	1.75	0.52
1:A1:564:ARG:HD3	3:C1:79:ALA:HB3	1.92	0.52
1:A1:84:PHE:CE1	14:A1:804:CLA:H91	2.45	0.52
1:A2:440:ILE:HD11	14:A2:1633:CLA:C1C	2.40	0.52
1:A3:686:SER:HB3	1:A3:734:HIS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:164:GLY:O	1:A4:168:MET:HG2	2.09	0.52
14:A5:821:CLA:HMB2	14:A5:825:CLA:HMA3	1.92	0.52
1:A1:544:PHE:CZ	14:B1:801:CLA:CBB	2.92	0.52
2:B1:353:GLN:NE2	14:B1:826:CLA:OBD	2.40	0.52
14:B1:833:CLA:CBB	14:B1:834:CLA:HMB2	2.39	0.52
2:B1:442:HIS:HB2	14:B1:834:CLA:NC	2.25	0.52
2:B2:122:TRP:CH2	14:B2:812:CLA:H201	2.44	0.52
2:B3:125:THR:HG21	14:B3:1820:CLA:HED1	1.92	0.52
2:B4:582:PHE:CE2	14:B4:831:CLA:HMD2	2.45	0.52
2:B5:453:GLU:HA	6:F5:48:LEU:HD22	1.91	0.52
2:B6:155:HIS:HE1	14:B6:811:CLA:C1A	2.23	0.52
6:F1:65:ILE:HD12	14:J1:102:CLA:HMB3	1.90	0.52
1:A2:118:TRP:HB3	16:J2:103:BCR:HC21	1.92	0.52
10:L6:49:GLU:HG2	14:L6:207:CLA:HED2	1.92	0.52
10:L6:50:VAL:O	10:L6:54:HIS:ND1	2.36	0.52
1:A1:43:GLN:OE1	5:E1:43:VAL:HG11	2.09	0.51
14:A1:820:CLA:HMB2	14:A1:824:CLA:HMA3	1.93	0.51
1:A4:436:HIS:CD2	1:A4:440:ILE:HG13	2.45	0.51
1:A5:100:TYR:HA	1:A5:144:PHE:CE1	2.45	0.51
1:A5:40:ARG:HD3	13:P5:61:ASP:HA	1.91	0.51
2:B1:278:ALA:HB2	14:B1:818:CLA:CBB	2.27	0.51
2:B1:45:ILE:CD1	14:B1:807:CLA:C2C	2.87	0.51
2:B2:267:LEU:HD21	2:B2:358:LEU:HD22	1.90	0.51
2:B3:487:ILE:HG12	14:B3:1837:CLA:HMD3	1.91	0.51
2:B6:179:ALA:HB2	2:B6:287:GLY:HA3	1.92	0.51
14:B6:819:CLA:HMB2	14:B6:824:CLA:HMA3	1.92	0.51
3:C3:11:ILE:HD11	13:P3:40:CYS:CA	2.34	0.51
4:D6:43:THR:O	4:D6:44:ALA:HB3	2.09	0.51
7:I6:30:LEU:O	7:I6:34:ILE:HG12	2.11	0.51
10:L1:62:TRP:HZ2	16:L1:203:BCR:C34	2.24	0.51
10:L4:62:TRP:CH2	14:L4:201:CLA:H11	2.43	0.51
14:B4:832:CLA:O1A	12:X4:12:ARG:HD3	2.09	0.51
1:A1:323:HIS:HB3	1:A1:328:ILE:HD11	1.91	0.51
1:A1:36:ARG:NH1	13:P1:70:ILE:HB	2.25	0.51
1:A1:694:ARG:HG2	2:B1:574:CYS:SG	2.50	0.51
1:A2:453:PHE:O	14:L2:202:CLA:CBB	2.57	0.51
14:A4:820:CLA:HMB2	14:A4:824:CLA:HMA3	1.92	0.51
2:B1:479:THR:O	2:B1:480:LEU:O	2.27	0.51
2:B1:177:HIS:HB3	14:B1:825:CLA:CED	2.40	0.51
14:B1:841:CLA:H171	7:I1:24:THR:CG2	2.40	0.51
2:B2:179:ALA:HB2	2:B2:287:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B2:807:CLA:C1A	14:B2:807:CLA:CGA	2.89	0.51
2:B3:172:SER:OG	14:B3:1814:CLA:O1D	2.29	0.51
2:B3:61:SER:OG	2:B3:138:ALA:O	2.28	0.51
2:B4:92:ASP:OD1	2:B4:94:GLN:NE2	2.38	0.51
14:B5:1831:CLA:H143	19:B5:1851:LMG:H231	1.92	0.51
2:B6:372:ALA:HB1	2:B6:731:LEU:HD11	1.93	0.51
2:B6:60:VAL:HG11	16:B6:845:BCR:H393	1.91	0.51
4:D3:59:ALA:N	4:D3:63:GLN:OE1	2.43	0.51
6:F3:65:ILE:HB	6:F3:66:PRO:HD3	1.92	0.51
8:J4:26:LEU:HD23	16:J4:103:BCR:HC7	1.92	0.51
8:J6:28:GLU:OE2	14:J6:1102:CLA:NA	2.43	0.51
14:L1:205:CLA:C1B	14:L1:206:CLA:HED1	2.40	0.51
10:L4:58:LEU:HD22	10:L4:85:LEU:CD1	2.41	0.51
1:A1:497:ALA:N	1:A1:498:PRO:CD	2.74	0.51
1:A1:447:VAL:HG21	14:A1:836:CLA:HMC3	1.91	0.51
1:A2:205:LEU:HD22	14:A2:1621:CLA:HMC2	1.92	0.51
1:A4:651:ARG:HD2	2:B4:639:ASN:HD21	1.75	0.51
14:B4:801:CLA:OBD	14:B4:803:CLA:HMB3	2.10	0.51
2:B4:651:VAL:HG13	14:B4:811:CLA:HHD	1.91	0.51
2:B6:694:ALA:HB1	14:L6:203:CLA:HMA1	1.91	0.51
2:B6:318:PHE:H	14:B6:822:CLA:C2B	2.23	0.51
2:B6:339:TRP:NE1	14:B6:824:CLA:C3B	2.68	0.51
14:B1:839:CLA:H203	6:F1:67:SER:HB3	1.92	0.51
7:I6:13:ILE:O	7:I6:17:VAL:HG23	2.11	0.51
1:A1:697:TRP:CZ2	15:A1:841:PQN:H2M3	2.46	0.51
1:A1:180:TYR:CE2	14:A1:810:CLA:C3D	2.94	0.51
14:A1:829:CLA:H111	17:A1:848:LHG:H202	1.93	0.51
1:A4:682:ILE:HD12	16:A4:849:BCR:H353	1.93	0.51
2:B1:279:ILE:CD1	14:B1:818:CLA:HBC2	2.40	0.51
2:B1:52:HIS:CD2	14:B1:807:CLA:HMA1	2.45	0.51
2:B1:532:GLY:HA2	2:B1:588:TRP:HZ3	1.74	0.51
2:B2:189:TRP:CZ3	2:B2:192:HIS:CD2	2.98	0.51
2:B3:52:HIS:CE1	14:B3:1807:CLA:CMA	2.93	0.51
2:B5:468:ALA:O	2:B5:482:SER:HB2	2.10	0.51
3:C6:14:THR:HG22	3:C6:27:MET:HG3	1.92	0.51
8:J6:27:ILE:HD13	16:J6:1105:BCR:C11	2.41	0.51
10:L5:15:GLY:O	10:L5:16:HIS:HB2	2.09	0.51
1:A1:581:PRO:HB3	2:B1:564:PRO:HB2	1.93	0.51
1:A5:472:GLN:OE1	1:A5:472:GLN:N	2.38	0.51
1:A6:543:ALA:HB1	14:A6:1637:CLA:HMB3	1.91	0.51
2:B1:350:LEU:HD13	14:B1:826:CLA:HED2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:59:TRP:CZ2	14:B1:829:CLA:HMB2	2.45	0.51
14:B1:809:CLA:CMD	7:I1:10:LEU:HD23	2.40	0.51
2:B2:278:ALA:HB2	14:B2:816:CLA:CBB	2.39	0.51
2:B2:503:TRP:CZ3	14:B2:816:CLA:H43	2.45	0.51
14:B2:837:CLA:H203	6:F2:67:SER:HB3	1.92	0.51
14:B3:1834:CLA:CBB	14:B3:1835:CLA:HMB2	2.40	0.51
2:B3:603:LYS:HD3	14:B3:1839:CLA:HBC1	1.93	0.51
2:B4:440:TYR:CE1	2:B4:524:LEU:HB3	2.44	0.51
2:B5:664:ALA:CB	14:B5:1805:CLA:CBB	2.88	0.51
2:B6:593:ILE:O	2:B6:597:THR:HG23	2.11	0.51
2:B6:654:TRP:CH2	14:B6:802:CLA:H72	2.46	0.51
4:D6:117:ARG:NH2	4:D6:138:PRO:OXT	2.43	0.51
6:F2:52:VAL:HG12	6:F2:54:ASP:HB2	1.93	0.51
14:B6:809:CLA:H201	7:I6:23:PRO:HA	1.93	0.51
10:L3:79:LEU:HD22	10:L3:136:PHE:CG	2.45	0.51
1:A1:36:ARG:CZ	13:P1:70:ILE:CG1	2.66	0.51
1:A2:741:ALA:HB2	16:A2:1652:BCR:H323	1.91	0.51
1:A2:433:VAL:HG21	14:A2:1623:CLA:H192	1.93	0.51
1:A3:305:ALA:O	1:A3:309:ILE:HG12	2.10	0.51
1:A5:198:ASN:HD21	1:A5:315:TYR:HB2	1.75	0.51
14:A6:1605:CLA:H71	16:A6:1645:BCR:H402	1.93	0.51
16:A6:1648:BCR:H362	14:A6:1651:CLA:C4	2.35	0.51
1:A6:366:LEU:HD11	14:A6:1619:CLA:H71	1.93	0.51
2:B4:117:SER:HB3	14:B4:829:CLA:HAA2	1.93	0.51
2:B6:61:SER:OG	2:B6:138:ALA:O	2.28	0.51
7:I6:22:MET:SD	7:I6:22:MET:C	2.89	0.51
8:J3:15:ALA:O	8:J3:19:MET:HB2	2.10	0.51
10:L2:54:HIS:HA	10:L2:57:PHE:CE2	2.45	0.51
12:X2:23:ASN:HD21	14:X2:1701:CLA:C1A	2.22	0.51
1:A1:577:PRO:O	1:A1:578:CYS:HB3	2.11	0.51
1:A1:302:LEU:HD11	14:A1:816:CLA:CBB	2.41	0.51
14:A1:826:CLA:HMB3	14:A1:832:CLA:H12	1.93	0.51
1:A4:546:ILE:O	1:A4:550:VAL:HG23	2.11	0.51
1:A5:79:HIS:NE2	14:A5:805:CLA:HMA1	2.26	0.51
14:A6:1633:CLA:HED2	10:L6:65:LEU:O	2.10	0.51
1:A6:269:THR:O	1:A6:270:PHE:HB2	2.11	0.51
1:A6:447:VAL:CG2	14:A6:1638:CLA:HMC3	2.41	0.51
2:B2:275:HIS:HB2	14:B2:816:CLA:CHB	2.41	0.51
1:A2:587:CYS:O	2:B2:675:GLY:N	2.44	0.51
2:B3:181:LEU:HD13	14:B3:1815:CLA:CHB	2.38	0.51
2:B4:738:LYS:O	2:B4:739:PHE:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:430:LEU:HD13	14:B4:802:CLA:HED3	1.91	0.51
2:B4:189:TRP:CD2	14:B4:820:CLA:HMD3	2.46	0.51
14:A5:802:CLA:OBD	14:B5:1803:CLA:HMB3	2.11	0.51
2:B6:526:HIS:HA	2:B6:529:ILE:HD12	1.93	0.51
14:B6:828:CLA:H51	16:B6:845:BCR:H392	1.91	0.51
3:C1:30:TRP:O	3:C1:36:GLY:HA2	2.10	0.51
3:C3:65:ARG:HG2	3:C3:67:TYR:CZ	2.46	0.51
6:F2:79:TRP:CH2	6:F2:120:ALA:HA	2.45	0.51
6:F4:70:PHE:CE1	16:F4:201:BCR:C10	2.87	0.51
14:B1:811:CLA:H201	7:I1:23:PRO:HA	1.93	0.51
14:A3:842:CLA:H172	8:J3:19:MET:HG3	1.92	0.51
1:A4:580:GLY:O	1:A4:586:THR:OG1	2.29	0.51
1:A5:341:HIS:HE1	17:A5:852:LHG:HC11	1.75	0.51
1:A5:681:PHE:CD2	16:A5:850:BCR:H363	2.46	0.51
2:B2:637:LEU:HD22	2:B2:730:PHE:HA	1.93	0.51
2:B3:42:TYR:CZ	2:B3:333:LEU:HD21	2.46	0.51
2:B4:195:HIS:CG	14:B4:816:CLA:CBC	2.93	0.51
1:A4:468:PHE:CZ	14:B4:811:CLA:CHC	2.94	0.51
2:B4:256:PHE:CD2	14:B4:819:CLA:HMB2	2.46	0.51
2:B6:537:THR:HG21	14:B6:825:CLA:HBB2	1.91	0.51
3:C1:2:HIS:NE2	3:C1:75:SER:HB2	2.26	0.51
16:I1:103:BCR:H383	10:L1:93:LEU:HD21	1.93	0.51
1:A1:90:MET:CE	14:A1:807:CLA:HED2	2.40	0.51
1:A4:502:ALA:N	1:A4:503:PRO:HD3	2.25	0.51
1:A5:592:TRP:CD1	14:A5:830:CLA:HMD1	2.46	0.51
14:A6:1627:CLA:HMB3	14:A6:1634:CLA:H12	1.93	0.51
14:B1:811:CLA:H203	7:I1:26:VAL:HG21	1.89	0.51
14:B3:1821:CLA:HMB2	14:B3:1826:CLA:HMA3	1.93	0.51
2:B4:243:PHE:CD1	2:B4:264:THR:HG21	2.45	0.51
2:B4:494:ASN:HD21	14:B4:837:CLA:CED	2.24	0.51
3:C1:80:TYR:HB3	4:D1:18:LEU:HD12	1.93	0.51
1:A6:582:GLY:CA	3:C6:48:VAL:O	2.59	0.51
2:B6:566:ASP:OD2	3:C6:65:ARG:NH2	2.43	0.51
10:L1:48:LEU:HD22	10:L1:52:MET:SD	2.51	0.51
1:A2:444:LEU:HB2	14:A2:1640:CLA:CBB	2.41	0.51
1:A4:403:PHE:HB3	14:A4:805:CLA:H112	1.93	0.51
14:A6:1621:CLA:HMB2	14:A6:1625:CLA:HMA3	1.93	0.51
14:B2:805:CLA:H151	14:B2:805:CLA:H102	1.93	0.51
14:B3:1842:CLA:CED	7:I3:31:PHE:HZ	2.24	0.51
14:B3:1842:CLA:HED3	7:I3:31:PHE:HZ	1.76	0.51
2:B3:455:GLN:OE1	2:B3:620:THR:OG1	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B6:636:GLN:HG3	2:B6:737:ALA:HB1	1.93	0.51
2:B6:527:HIS:CD2	16:B6:850:BCR:H322	2.45	0.51
6:F5:65:ILE:HB	6:F5:66:PRO:HD3	1.93	0.51
8:J3:26:LEU:HD23	16:J3:103:BCR:HC7	1.93	0.51
10:L3:54:HIS:HA	10:L3:57:PHE:CE2	2.46	0.51
10:L6:33:ASN:N	10:L6:33:ASN:HD22	2.09	0.51
11:M5:17:LEU:HB3	11:M5:18:PRO:HD3	1.93	0.51
3:C2:11:ILE:CD1	13:P2:40:CYS:HA	2.40	0.51
14:A1:804:CLA:H71	16:A1:844:BCR:H402	1.93	0.50
1:A2:362:MET:HA	1:A2:365:SER:OG	2.11	0.50
1:A2:518:VAL:HG23	1:A2:525:ALA:HB3	1.93	0.50
1:A3:502:ALA:N	1:A3:503:PRO:HD3	2.25	0.50
14:A3:805:CLA:H71	16:A3:849:BCR:H402	1.93	0.50
14:A3:827:CLA:HMB3	14:A3:835:CLA:H12	1.92	0.50
1:A4:259:GLY:C	1:A4:261:PHE:H	2.14	0.50
2:B1:521:GLY:O	2:B1:525:VAL:HG22	2.11	0.50
2:B1:652:TRP:CZ2	2:B1:732:ILE:HG21	2.46	0.50
14:B1:801:CLA:OBD	14:B1:804:CLA:HMB3	2.10	0.50
2:B1:595:TRP:HZ2	14:B1:805:CLA:NB	2.09	0.50
2:B4:347:ILE:O	2:B4:351:VAL:HG23	2.10	0.50
2:B4:467:GLN:NE2	14:B4:839:CLA:HMD1	2.26	0.50
2:B5:503:TRP:CE3	14:B5:1819:CLA:H11	2.46	0.50
2:B6:256:PHE:HB2	14:B6:816:CLA:O1D	2.10	0.50
2:B6:7:PHE:HB2	2:B6:33:HIS:CG	2.46	0.50
2:B6:599:TYR:CZ	14:B6:837:CLA:CBC	2.94	0.50
3:C4:77:GLY:HA2	4:D4:60:ARG:CZ	2.40	0.50
9:K1:40:GLY:O	9:K1:41:PRO:C	2.49	0.50
14:L1:207:CLA:HMD1	14:B3:1812:CLA:H203	1.93	0.50
14:B1:854:CLA:CBA	10:L2:148:ILE:HG23	2.41	0.50
10:L3:7:PRO:HB3	10:L3:12:PRO:HA	1.92	0.50
10:L3:48:LEU:HD22	10:L3:52:MET:SD	2.51	0.50
1:A1:356:LEU:O	1:A1:360:LEU:HB2	2.11	0.50
14:A2:1607:CLA:H71	16:A2:1649:BCR:H402	1.93	0.50
14:A2:1616:CLA:HBA2	14:A2:1618:CLA:HMB3	1.93	0.50
1:A2:313:HIS:CE1	16:A2:1647:BCR:H363	2.46	0.50
1:A5:513:PHE:CE1	14:A5:827:CLA:HMC3	2.47	0.50
1:A6:106:ASP:N	1:A6:107:PRO:HD3	2.26	0.50
1:A6:531:LEU:HA	1:A6:535:ASP:OD1	2.11	0.50
2:B1:30:PHE:CD1	14:B1:807:CLA:HMC2	2.46	0.50
2:B2:339:TRP:NE1	14:B2:823:CLA:C3B	2.72	0.50
2:B4:537:THR:HG21	14:B4:827:CLA:CBB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B5:436:THR:HG22	14:B5:1803:CLA:H192	1.94	0.50
4:D2:32:THR:HA	4:D2:52:GLY:O	2.12	0.50
1:A6:709:ASN:HB3	6:F6:136:ILE:HG23	1.92	0.50
7:I1:16:PRO:HB3	7:I1:20:TRP:CZ3	2.46	0.50
11:M4:12:LEU:HB3	16:M4:101:BCR:C21	2.41	0.50
1:A2:173:LEU:HD21	14:A2:1611:CLA:H201	1.93	0.50
1:A2:440:ILE:CD1	14:A2:1633:CLA:C1C	2.89	0.50
1:A3:269:THR:O	1:A3:270:PHE:HB2	2.12	0.50
1:A3:468:PHE:CZ	14:B3:1811:CLA:CHC	2.94	0.50
14:A4:820:CLA:CMD	14:A4:821:CLA:HBB1	2.41	0.50
1:A4:90:MET:CE	14:A4:807:CLA:HED2	2.40	0.50
2:B1:528:ALA:HB1	14:B1:804:CLA:H172	1.94	0.50
16:B2:843:BCR:H382	16:B2:843:BCR:H23C	1.93	0.50
2:B3:192:HIS:HB2	14:B3:1816:CLA:C4B	2.41	0.50
2:B3:598:PHE:HE1	14:B3:1803:CLA:HED2	1.76	0.50
2:B4:256:PHE:CE1	14:B4:819:CLA:CAB	2.86	0.50
2:B5:141:LEU:HD23	2:B5:144:LEU:HD12	1.94	0.50
2:B6:537:THR:CG2	14:B6:825:CLA:CBB	2.87	0.50
4:D2:50:ARG:HG2	4:D2:54:ASN:HD21	1.75	0.50
4:D3:32:THR:HA	4:D3:52:GLY:O	2.11	0.50
1:A1:682:ILE:HD12	16:A1:847:BCR:H353	1.94	0.50
1:A2:79:HIS:CE1	14:A2:1607:CLA:CMA	2.95	0.50
1:A2:302:LEU:HD13	14:A2:1617:CLA:HMC1	1.93	0.50
16:A4:849:BCR:H362	14:B4:804:CLA:C4	2.35	0.50
2:B1:128:MET:HE1	2:B1:134:LEU:HA	1.93	0.50
2:B1:463:ALA:HB2	14:B1:839:CLA:CGD	2.41	0.50
14:B1:854:CLA:CBB	7:I1:19:CYS:HB3	2.42	0.50
2:B2:136:GLN:NE2	14:B2:813:CLA:HBD	2.26	0.50
2:B2:369:THR:HA	2:B2:735:THR:HG21	1.93	0.50
2:B2:589:MET:O	2:B2:593:ILE:HG12	2.11	0.50
2:B5:92:ASP:HB3	2:B5:95:PHE:CD2	2.46	0.50
2:B6:438:GLY:C	14:B6:833:CLA:HBB1	2.31	0.50
4:D3:2:THR:HG21	4:D3:91:THR:HB	1.92	0.50
6:F1:73:ILE:O	6:F1:76:TRP:HB3	2.10	0.50
6:F1:99:ILE:O	8:J1:11:ALA:N	2.37	0.50
7:I5:9:PHE:CE1	7:I5:10:LEU:HD13	2.47	0.50
14:A1:838:CLA:CMC	14:B1:802:CLA:H71	2.42	0.50
1:A4:391:LEU:O	1:A4:395:THR:HG23	2.10	0.50
1:A4:581:PRO:CG	3:C4:68:LEU:HD11	2.41	0.50
14:A4:817:CLA:H41	14:A4:833:CLA:HAA2	1.94	0.50
1:A6:77:PHE:CZ	14:A6:1613:CLA:HED1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A6:697:TRP:CH2	15:A6:1642:PQN:H2M3	2.47	0.50
14:B2:809:CLA:HAA2	10:L2:67:PRO:HG3	1.93	0.50
2:B2:117:SER:O	14:B2:827:CLA:HED3	2.11	0.50
2:B3:713:LEU:HD23	19:B3:1850:LMG:H122	1.93	0.50
2:B4:652:TRP:CH2	14:B4:810:CLA:HBC2	2.47	0.50
2:B4:667:PHE:CB	14:B4:805:CLA:HMC3	2.42	0.50
14:B4:810:CLA:C1A	14:B4:810:CLA:CGA	2.90	0.50
16:B5:1846:BCR:H382	16:B5:1846:BCR:H23C	1.94	0.50
2:B6:135:TYR:O	2:B6:139:ILE:HG12	2.11	0.50
2:B6:52:HIS:ND1	14:B6:806:CLA:O1A	2.44	0.50
3:C5:6:ILE:HD13	3:C5:40:SER:O	2.11	0.50
4:D2:39:PHE:CE2	4:D2:47:ALA:HB3	2.46	0.50
5:E3:44:ASN:OD1	5:E3:55:VAL:HB	2.12	0.50
2:B2:551:LYS:HD2	6:F2:139:SER:HA	1.94	0.50
6:F4:77:ILE:HG12	14:F4:202:CLA:C4D	2.41	0.50
10:L2:61:PRO:HB3	14:L2:207:CLA:HBB1	1.92	0.50
1:A2:83:VAL:HG11	14:A2:1607:CLA:H72	1.94	0.50
14:A2:1623:CLA:CMB	14:A2:1627:CLA:HMA3	2.42	0.50
14:A2:1629:CLA:HMB3	14:A2:1636:CLA:H12	1.94	0.50
1:A2:497:ALA:N	1:A2:498:PRO:CD	2.75	0.50
14:A3:830:CLA:H111	17:A3:853:LHG:H202	1.93	0.50
1:A6:433:VAL:HG21	14:A6:1621:CLA:H192	1.92	0.50
1:A6:444:LEU:HB2	14:A6:1638:CLA:CBB	2.41	0.50
2:B1:208:TRP:NE1	14:B1:815:CLA:CAD	2.75	0.50
2:B1:284:ILE:O	2:B1:288:HIS:ND1	2.42	0.50
2:B1:72:ASN:HB3	2:B1:86:ILE:HD12	1.93	0.50
2:B1:53:LEU:HD13	14:B1:807:CLA:CBA	2.42	0.50
2:B6:142:LEU:HD23	11:M6:14:ILE:CG2	2.42	0.50
16:F4:204:BCR:H23C	8:J4:40:PRO:HD2	1.94	0.50
10:L5:62:TRP:CE2	14:L5:203:CLA:C1	2.95	0.50
1:A2:297:THR:O	1:A2:300:HIS:HB3	2.12	0.50
1:A3:444:LEU:HD13	14:A3:839:CLA:HBB1	1.93	0.50
14:A3:834:CLA:C1	10:L3:62:TRP:CE2	2.95	0.50
2:B1:65:PHE:CD2	14:B1:809:CLA:C4C	2.95	0.50
2:B3:718:HIS:HE1	14:B3:1843:CLA:C4D	2.24	0.50
2:B5:529:ILE:O	2:B5:533:LEU:HG	2.12	0.50
2:B5:554:PRO:HD2	3:C5:61:PHE:CE1	2.46	0.50
10:L5:20:PRO:HB2	14:L5:202:CLA:HMD1	1.92	0.50
11:M4:21:LEU:HD21	14:A6:1601:CLA:CMA	2.41	0.50
14:A1:805:CLA:H3A	14:A1:829:CLA:HAB	1.94	0.50
1:A2:385:THR:HG23	1:A2:523:LYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:216:GLN:NE2	1:A5:297:THR:OG1	2.41	0.50
1:A5:683:TRP:O	1:A5:686:SER:OG	2.27	0.50
2:B1:229:TRP:C	14:B1:817:CLA:H3A	2.32	0.50
2:B1:346:VAL:CG2	16:B1:847:BCR:H362	2.41	0.50
2:B1:423:SER:C	14:B1:803:CLA:HED2	2.32	0.50
2:B3:467:GLN:HE22	14:B3:1839:CLA:HMD1	1.75	0.50
2:B4:234:GLN:O	2:B4:236:PRO:HD3	2.12	0.50
2:B5:622:LEU:HD11	14:B5:1803:CLA:H202	1.92	0.50
2:B5:103:PHE:CZ	2:B5:651:VAL:HG22	2.47	0.50
2:B5:718:HIS:CE1	14:B5:1843:CLA:C4D	2.94	0.50
5:E4:7:VAL:O	5:E4:20:VAL:HA	2.12	0.50
2:B5:20:ILE:HG12	7:I5:34:ILE:HD12	1.94	0.50
8:J2:28:GLU:OE2	14:J2:101:CLA:NA	2.45	0.50
8:J4:27:ILE:HG21	16:J4:104:BCR:H343	1.92	0.50
10:L1:105:GLY:O	10:L1:106:SER:HB2	2.11	0.50
10:L6:134:VAL:HG23	16:L6:201:BCR:H403	1.94	0.50
1:A1:543:ALA:HB1	14:A1:835:CLA:HMB3	1.94	0.50
2:B1:532:GLY:O	2:B1:536:THR:OG1	2.16	0.50
16:B1:844:BCR:H23C	16:B1:844:BCR:H382	1.94	0.50
2:B2:347:ILE:O	2:B2:351:VAL:HG23	2.12	0.50
2:B3:434:PHE:CE2	14:B3:1802:CLA:H2	2.47	0.50
2:B3:564:PRO:O	2:B3:565:CYS:HB3	2.12	0.50
2:B3:599:TYR:CZ	14:B3:1839:CLA:CB	2.95	0.50
2:B3:682:GLU:HG2	3:C3:80:TYR:CE2	2.47	0.50
14:B4:832:CLA:HMB2	14:B4:833:CLA:C2D	2.42	0.50
2:B5:181:LEU:HG	14:B5:1815:CLA:H43	1.94	0.50
2:B5:189:TRP:HA	14:B5:1816:CLA:HBB1	1.92	0.50
2:B5:537:THR:HG21	14:B5:1827:CLA:HBB2	1.94	0.50
6:F2:69:LEU:CB	14:F2:204:CLA:CBB	2.83	0.50
2:B1:4:PHE:CD2	7:I1:34:ILE:HG22	2.47	0.50
10:L5:19:THR:OG1	10:L5:22:SER:N	2.37	0.50
14:B3:1841:CLA:HBC2	14:X3:102:CLA:HBC3	1.94	0.50
1:A1:502:ALA:N	1:A1:503:PRO:HD3	2.27	0.49
14:A1:803:CLA:H2	14:A1:810:CLA:H92	1.93	0.49
14:A2:1601:CLA:HAC2	14:L2:206:CLA:H151	1.94	0.49
1:A2:194:GLU:CG	1:A2:315:TYR:HB3	2.42	0.49
1:A3:657:GLN:HA	1:A3:750:ARG:NH1	2.27	0.49
14:A3:821:CLA:HMB2	14:A3:825:CLA:HMA3	1.94	0.49
1:A3:313:HIS:NE2	16:A3:847:BCR:H363	2.26	0.49
14:A4:826:CLA:HMB3	14:A4:833:CLA:H12	1.94	0.49
1:A4:99:ASN:HB3	1:A4:134:PHE:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A5:827:CLA:HBB1	14:A5:834:CLA:HMA2	1.94	0.49
2:B1:300:ILE:HA	2:B1:303:MET:SD	2.52	0.49
2:B1:458:ILE:N	2:B1:458:ILE:HD12	2.27	0.49
2:B1:361:TYR:CE2	14:B1:819:CLA:HAA2	2.47	0.49
14:B1:820:CLA:HMB2	14:B1:825:CLA:HMA3	1.94	0.49
2:B1:25:ALA:CB	19:B1:850:LMG:O7	2.60	0.49
14:B3:1839:CLA:H101	12:X3:23:ASN:HA	1.94	0.49
2:B4:184:VAL:HG12	16:B4:846:BCR:H352	1.93	0.49
2:B5:439:LEU:HD22	2:B5:456:ILE:HG21	1.94	0.49
2:B6:339:TRP:CZ2	14:B6:824:CLA:HAB	2.47	0.49
6:F4:63:PHE:HE1	16:F4:204:BCR:C10	2.25	0.49
8:J1:27:ILE:CD1	16:J1:104:BCR:C11	2.86	0.49
1:A2:461:HIS:CD2	1:A2:475:PHE:CE1	3.00	0.49
1:A4:741:ALA:HB2	16:A4:849:BCR:H323	1.93	0.49
14:A4:804:CLA:H71	16:A4:846:BCR:H402	1.94	0.49
1:A5:502:ALA:N	1:A5:503:PRO:HD3	2.27	0.49
1:A5:686:SER:HB3	1:A5:734:HIS:CB	2.42	0.49
14:A5:804:CLA:H2	14:A5:811:CLA:H92	1.93	0.49
14:A6:1633:CLA:HED3	10:L6:69:ARG:HH21	1.77	0.49
2:B1:182:PHE:CE2	14:B1:814:CLA:H61	2.47	0.49
2:B1:430:LEU:HB3	14:B1:833:CLA:HED3	1.92	0.49
2:B1:660:HIS:CD2	14:B1:804:CLA:CHB	2.96	0.49
2:B2:137:GLY:CA	16:B2:844:BCR:H381	2.42	0.49
2:B3:153:TRP:CZ3	14:B3:1801:CLA:H62	2.46	0.49
2:B3:339:TRP:HZ2	14:B3:1826:CLA:HAB	1.77	0.49
2:B3:600:TRP:CE2	2:B3:604:HIS:CE1	3.00	0.49
2:B4:229:TRP:CE3	14:B4:818:CLA:CMB	2.95	0.49
2:B4:660:HIS:HD2	14:B4:801:CLA:O2D	1.94	0.49
2:B6:386:MET:CE	16:B6:847:BCR:H361	2.42	0.49
1:A4:423:ALA:CA	4:D4:38:VAL:HG11	2.41	0.49
10:L1:62:TRP:HZ2	16:L1:203:BCR:H342	1.77	0.49
16:L2:201:BCR:H341	14:L2:207:CLA:HBC1	1.95	0.49
1:A4:36:ARG:HH11	13:P4:67:ASP:HA	1.77	0.49
12:X4:23:ASN:OD1	14:X4:102:CLA:CHB	2.60	0.49
14:A1:817:CLA:H41	14:A1:832:CLA:HAA2	1.93	0.49
1:A2:502:ALA:N	1:A2:503:PRO:HD3	2.27	0.49
14:A3:818:CLA:H41	14:A3:835:CLA:HAA2	1.95	0.49
2:B1:660:HIS:NE2	14:B1:804:CLA:C4A	2.75	0.49
2:B2:360:PRO:HG3	14:B2:817:CLA:HBA2	1.93	0.49
2:B3:189:TRP:CZ3	2:B3:192:HIS:CD2	3.00	0.49
2:B3:447:VAL:HG11	2:B3:621:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B5:1832:CLA:HMB2	14:B5:1833:CLA:C2D	2.42	0.49
4:D1:129:LYS:HE2	4:D1:130:PHE:CE1	2.47	0.49
4:D4:32:THR:HA	4:D4:52:GLY:O	2.12	0.49
6:F3:63:PHE:C	6:F3:66:PRO:HD2	2.32	0.49
6:F6:76:TRP:CD2	14:F6:202:CLA:HAA2	2.48	0.49
10:L2:36:ALA:HB2	14:L2:206:CLA:HMD1	1.94	0.49
10:L3:20:PRO:O	10:L3:24:SER:HB3	2.13	0.49
1:A4:453:PHE:C	14:L4:201:CLA:HBB2	2.31	0.49
10:L5:62:TRP:CE2	14:L5:203:CLA:H12	2.47	0.49
10:L5:48:LEU:HD13	14:L5:204:CLA:CED	2.42	0.49
1:A2:120:ILE:C	1:A2:122:GLY:H	2.15	0.49
14:A2:1620:CLA:H41	14:A2:1636:CLA:HAA2	1.95	0.49
14:A3:802:CLA:OBD	14:B3:1803:CLA:HMB3	2.11	0.49
1:A3:433:VAL:HG21	14:A3:821:CLA:H192	1.93	0.49
1:A5:683:TRP:CE2	14:A5:801:CLA:HBA2	2.48	0.49
1:A6:678:GLY:O	1:A6:681:PHE:HB3	2.13	0.49
2:B1:622:LEU:CG	14:B1:805:CLA:H11	2.43	0.49
14:B1:831:CLA:HMB2	14:B1:832:CLA:C2D	2.42	0.49
2:B1:438:GLY:C	14:B1:834:CLA:HBB1	2.32	0.49
2:B2:277:LEU:HD11	14:B2:815:CLA:CBB	2.42	0.49
2:B3:277:LEU:HD13	14:B3:1817:CLA:CMC	2.42	0.49
14:B4:841:CLA:HBC2	14:X4:102:CLA:HBC3	1.94	0.49
2:B5:42:TYR:CD2	2:B5:167:PHE:HB3	2.47	0.49
2:B6:589:MET:HE2	2:B6:590:LEU:HD23	1.94	0.49
3:C1:50:CYS:HG	18:C1:101:SF4:FE1	1.26	0.49
3:C6:28:VAL:HG12	4:D6:109:ARG:HB3	1.94	0.49
4:D6:39:PHE:CE1	4:D6:67:LEU:HD11	2.47	0.49
6:F5:53:VAL:HG12	6:F5:63:PHE:HB2	1.94	0.49
8:J6:27:ILE:CG2	16:J6:1105:BCR:H343	2.43	0.49
10:L4:57:PHE:CD1	10:L4:57:PHE:C	2.85	0.49
1:A3:257:ASP:OD1	1:A3:258:TRP:N	2.45	0.49
14:A3:814:CLA:HBA2	14:A3:816:CLA:HMB3	1.94	0.49
1:A5:686:SER:HB3	1:A5:734:HIS:HB2	1.94	0.49
14:A5:818:CLA:H41	14:A5:834:CLA:HAA2	1.93	0.49
1:A6:90:MET:CE	14:A6:1608:CLA:HED2	2.42	0.49
2:B1:275:HIS:CE1	14:B1:818:CLA:C4C	2.95	0.49
1:A2:597:LEU:HD21	2:B2:672:SER:HB3	1.94	0.49
2:B4:493:PRO:HG3	14:B4:838:CLA:C1D	2.43	0.49
14:B4:816:CLA:HAB	14:B4:830:CLA:H13	1.94	0.49
2:B6:155:HIS:CE1	14:B6:811:CLA:NA	2.81	0.49
2:B6:267:LEU:HD13	14:B6:817:CLA:H2A	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C3:25:LEU:HA	3:C3:40:SER:O	2.12	0.49
5:E4:44:ASN:OD1	5:E4:55:VAL:HB	2.13	0.49
10:L4:105:GLY:O	10:L4:106:SER:HB2	2.13	0.49
14:L6:206:CLA:H43	14:L6:206:CLA:HMB2	1.95	0.49
5:E2:57:THR:CG2	13:P2:42:ALA:CB	2.90	0.49
1:A1:120:ILE:C	1:A1:122:GLY:H	2.16	0.49
1:A1:682:ILE:HD11	16:A1:847:BCR:C15	2.42	0.49
1:A1:440:ILE:HG12	14:A1:830:CLA:CHC	2.42	0.49
1:A2:300:HIS:O	1:A2:304:ILE:HG12	2.13	0.49
1:A2:588:GLN:HA	1:A2:593:ASP:OD2	2.12	0.49
14:A4:805:CLA:H3A	14:A4:829:CLA:HAB	1.93	0.49
14:A4:813:CLA:HBA2	14:A4:815:CLA:HMB3	1.95	0.49
14:A6:1629:CLA:HMB1	14:A6:1629:CLA:HBB1	1.94	0.49
1:A6:275:TYR:CZ	14:A6:1615:CLA:HMD2	2.47	0.49
1:A6:359:ASN:HD22	1:A6:359:ASN:N	2.10	0.49
2:B1:376:THR:HG23	2:B1:597:THR:HG21	1.93	0.49
2:B1:439:LEU:N	14:B1:834:CLA:HBB1	2.28	0.49
2:B2:181:LEU:CD1	14:B2:812:CLA:H43	2.43	0.49
2:B2:431:PHE:CZ	16:B2:850:BCR:HC41	2.48	0.49
2:B3:664:ALA:C	14:B3:1805:CLA:HBB1	2.32	0.49
2:B3:682:GLU:HG2	3:C3:80:TYR:HE2	1.77	0.49
2:B4:533:LEU:O	2:B4:537:THR:OG1	2.20	0.49
2:B4:641:TYR:HB2	2:B4:646:THR:HG22	1.94	0.49
2:B4:116:TYR:CD1	14:B4:810:CLA:CMD	2.96	0.49
2:B4:651:VAL:HG11	14:B4:811:CLA:HMD2	1.94	0.49
14:B4:812:CLA:H101	14:L6:208:CLA:H91	1.95	0.49
2:B4:176:HIS:CE1	14:B4:815:CLA:HMC2	2.47	0.49
2:B5:535:THR:HG23	14:B5:1802:CLA:HBD	1.95	0.49
14:B5:1821:CLA:HMB2	14:B5:1826:CLA:HMA3	1.94	0.49
1:A1:572:LEU:HD21	3:C1:52:ARG:CZ	2.42	0.49
2:B1:554:PRO:HD2	3:C1:61:PHE:CZ	2.48	0.49
4:D6:50:ARG:H	4:D6:54:ASN:HD21	1.60	0.49
5:E3:7:VAL:O	5:E3:20:VAL:HA	2.12	0.49
7:I2:13:ILE:O	7:I2:17:VAL:HG23	2.13	0.49
7:I6:9:PHE:CE1	7:I6:10:LEU:HD13	2.46	0.49
9:K5:65:PHE:O	9:K5:69:LEU:CB	2.60	0.49
14:L4:205:CLA:H13	7:I5:20:TRP:CE3	2.42	0.49
14:B5:1841:CLA:HBC2	14:X5:101:CLA:HBC3	1.94	0.49
1:A1:744:TRP:HB2	14:A1:827:CLA:HBB1	1.94	0.49
14:A2:1608:CLA:H3A	14:A2:1632:CLA:HAB	1.93	0.49
14:A6:1614:CLA:HBA2	14:A6:1616:CLA:HMB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:382:ALA:O	2:B1:386:MET:HG2	2.13	0.49
2:B1:48:SER:HB3	14:B1:807:CLA:HBB1	1.95	0.49
2:B2:42:TYR:CE2	2:B2:333:LEU:HD21	2.48	0.49
16:B4:846:BCR:H23C	16:B4:846:BCR:H382	1.94	0.49
14:B6:808:CLA:CGA	14:B6:808:CLA:C1A	2.91	0.49
14:A3:803:CLA:H142	8:J3:19:MET:HB3	1.95	0.49
6:F4:69:LEU:HB2	14:J4:102:CLA:CBB	2.42	0.49
10:L2:79:LEU:HD11	10:L2:83:ILE:HD11	1.95	0.49
14:L4:203:CLA:C1B	14:L4:204:CLA:HED1	2.43	0.49
5:E2:39:ARG:NH2	13:P2:24:TYR:OH	2.46	0.49
3:C6:18:ARG:NE	13:P6:97:TYR:CE2	2.81	0.49
3:C6:18:ARG:NH2	13:P6:97:TYR:CE2	2.81	0.49
14:B1:840:CLA:HBC2	14:X1:1701:CLA:HBC3	1.94	0.49
1:A1:482:LEU:HB2	1:A1:533:THR:HG23	1.93	0.49
14:A2:1623:CLA:CMD	14:A2:1624:CLA:HBB1	2.42	0.49
1:A2:40:ARG:HG3	13:P2:60:SER:HB2	1.94	0.49
1:A3:564:ARG:NH2	4:D3:14:THR:O	2.46	0.49
1:A5:741:ALA:HB2	16:A5:850:BCR:H323	1.95	0.49
14:A6:1618:CLA:H41	14:A6:1634:CLA:HAA2	1.95	0.49
2:B1:625:TRP:HB3	14:B1:804:CLA:H91	1.94	0.49
2:B2:658:PHE:HE2	2:B2:725:LEU:CD1	2.25	0.49
14:B2:829:CLA:HMB2	14:B2:830:CLA:C2D	2.43	0.49
2:B3:727:TYR:HB2	14:B3:1803:CLA:HED3	1.95	0.49
2:B4:133:ASP:O	2:B4:136:GLN:HG2	2.11	0.49
2:B5:710:GLN:HG3	19:B5:1851:LMG:H111	1.93	0.49
2:B6:423:SER:HB2	14:B6:803:CLA:HED2	1.94	0.49
4:D1:30:THR:HA	4:D1:54:ASN:O	2.13	0.49
6:F2:88:VAL:HG11	6:F2:97:LYS:CB	2.43	0.49
6:F3:88:VAL:HG11	6:F3:97:LYS:CB	2.43	0.49
6:F5:88:VAL:O	6:F5:89:ARG:C	2.49	0.49
14:A3:843:CLA:H171	10:L3:85:LEU:HD11	1.94	0.49
10:L6:65:LEU:HA	10:L6:69:ARG:HD3	1.95	0.49
13:P4:27:ASP:OD1	13:P4:41:ARG:NH2	2.46	0.49
1:A1:259:GLY:C	1:A1:261:PHE:H	2.16	0.49
1:A2:259:GLY:C	1:A2:261:PHE:H	2.16	0.49
1:A2:28:TRP:HE1	14:A2:1613:CLA:CHB	2.25	0.49
1:A3:356:LEU:O	1:A3:360:LEU:HB2	2.12	0.49
1:A3:577:PRO:O	1:A3:578:CYS:HB3	2.13	0.49
1:A5:548:VAL:HG11	1:A5:601:TRP:CZ2	2.48	0.49
14:A5:806:CLA:H3A	14:A5:830:CLA:HAB	1.95	0.49
2:B1:233:ALA:HB1	14:B1:817:CLA:HED3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:682:GLU:HG2	3:C1:80:TYR:CE2	2.47	0.49
2:B2:376:THR:HG23	2:B2:597:THR:HG21	1.94	0.49
2:B2:65:PHE:CE2	14:B2:806:CLA:C4C	2.96	0.49
2:B2:275:HIS:HE1	14:B2:816:CLA:C4C	2.26	0.49
2:B3:360:PRO:HB2	14:B3:1820:CLA:HAA2	1.95	0.49
16:B6:844:BCR:H382	16:B6:844:BCR:H23C	1.93	0.49
16:B6:850:BCR:H331	16:B6:850:BCR:HC8	1.95	0.49
6:F2:65:ILE:HG23	14:F2:204:CLA:C2B	2.42	0.49
7:I4:13:ILE:O	7:I4:16:PRO:HD2	2.13	0.49
10:L3:58:LEU:HD22	10:L3:85:LEU:HD12	1.94	0.49
7:I4:1:MET:HG3	10:L6:150:THR:O	2.13	0.49
14:B3:1806:CLA:H2	11:M3:26:SER:HB2	1.94	0.49
1:A1:741:ALA:HB2	16:A1:847:BCR:H323	1.94	0.49
1:A2:353:HIS:CD2	14:A2:1607:CLA:HBC1	2.47	0.49
1:A2:272:TRP:CZ3	14:A2:1619:CLA:H2	2.48	0.49
1:A2:47:TRP:CZ3	1:A2:51:LEU:HD12	2.47	0.49
1:A4:385:THR:HG23	1:A4:523:LYS:HB2	1.94	0.49
14:A4:820:CLA:HMD1	14:A4:821:CLA:HBB1	1.95	0.49
2:B1:298:HIS:CE1	14:B1:823:CLA:HMD1	2.48	0.49
2:B1:496:GLY:CA	14:B1:836:CLA:HED2	2.43	0.49
14:B2:806:CLA:HBC2	11:M2:12:LEU:HD23	1.95	0.49
2:B2:150:PHE:CD2	14:B2:810:CLA:HBC3	2.48	0.49
14:B3:1806:CLA:H2	11:M3:26:SER:CB	2.42	0.49
2:B5:720:SER:HB2	19:B5:1851:LMG:H391	1.95	0.49
2:B5:232:TYR:CD2	2:B5:253:ILE:HD11	2.47	0.49
3:C4:65:ARG:HG2	3:C4:67:TYR:CZ	2.48	0.49
3:C5:45:GLU:OE1	3:C5:45:GLU:N	2.45	0.49
3:C5:52:ARG:HA	3:C5:55:THR:HB	1.95	0.49
4:D6:32:THR:HA	4:D6:52:GLY:O	2.13	0.49
7:I4:12:TRP:CE2	10:L6:149:MET:HG3	2.48	0.49
8:J1:31:ARG:NH1	14:J1:101:CLA:HED2	2.27	0.49
14:A2:1601:CLA:HMD2	10:L2:21:ILE:CD1	2.43	0.49
5:E2:3:ARG:HH12	13:P2:31:GLU:CB	2.25	0.49
1:A1:375:TYR:CE1	1:A1:376:ALA:HB2	2.48	0.48
1:A4:356:LEU:O	1:A4:360:LEU:HB2	2.12	0.48
1:A4:215:HIS:HB2	14:A4:813:CLA:CHC	2.43	0.48
1:A5:196:MET:HE2	14:A5:813:CLA:HBC2	1.93	0.48
14:A5:828:CLA:H93	16:J5:103:BCR:H20C	1.95	0.48
14:A6:1622:CLA:HBA2	14:A6:1622:CLA:H3A	1.51	0.48
2:B1:433:GLY:HA2	2:B1:531:LEU:HD22	1.93	0.48
2:B2:456:ILE:HG22	2:B2:458:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:680:HIS:CD2	14:B2:802:CLA:O1D	2.66	0.48
1:A3:651:ARG:HB2	2:B3:638:ILE:HG23	1.94	0.48
2:B4:414:VAL:HG11	16:B4:848:BCR:H401	1.94	0.48
2:B6:433:GLY:HA2	2:B6:531:LEU:HD22	1.93	0.48
2:B6:727:TYR:HB2	14:B6:804:CLA:HED3	1.95	0.48
5:E2:24:ALA:O	5:E2:25:SER:HB3	2.12	0.48
5:E2:37:ILE:HG21	13:P2:41:ARG:HD3	1.95	0.48
14:L3:203:CLA:C1B	14:L3:204:CLA:HED1	2.43	0.48
10:L4:41:LEU:HD13	10:L4:45:LEU:HD23	1.95	0.48
7:I4:25:VAL:CG2	14:L6:206:CLA:H62	2.43	0.48
13:P1:27:ASP:OD1	13:P1:41:ARG:NH2	2.46	0.48
1:A1:445:ASN:ND2	14:B1:806:CLA:HED2	2.28	0.48
1:A1:473:ASP:HA	10:L1:69:ARG:HH22	1.79	0.48
1:A2:543:ALA:HB1	14:A2:1639:CLA:HMB3	1.95	0.48
1:A2:694:ARG:NH1	2:B2:572:GLY:O	2.46	0.48
1:A5:360:LEU:HD11	14:A5:830:CLA:HBB1	1.95	0.48
14:A5:821:CLA:CMB	14:A5:825:CLA:HMA3	2.43	0.48
14:A6:1651:CLA:H61	14:A6:1651:CLA:H41	1.65	0.48
2:B1:122:TRP:CZ2	14:B1:814:CLA:C19	2.93	0.48
2:B2:166:TRP:CZ2	14:B2:812:CLA:CAC	2.94	0.48
2:B2:641:TYR:OH	2:B2:657:LEU:HD12	2.13	0.48
2:B3:300:ILE:HD13	14:B3:1826:CLA:HAC1	1.95	0.48
16:B3:1846:BCR:H23C	16:B3:1846:BCR:H382	1.94	0.48
2:B4:481:LEU:CD1	14:B4:836:CLA:HED3	2.43	0.48
14:B5:1804:CLA:H41	14:B5:1804:CLA:H61	1.64	0.48
14:B6:839:CLA:HBC2	14:X6:1701:CLA:HBC3	1.94	0.48
3:C5:17:VAL:CA	3:C5:25:LEU:HD12	2.44	0.48
3:C2:7:TYR:CE1	4:D2:119:ILE:HD12	2.48	0.48
6:F4:76:TRP:CD1	14:F4:202:CLA:HBD	2.48	0.48
14:A5:803:CLA:H142	8:J5:19:MET:HB3	1.95	0.48
1:A1:360:LEU:HD13	14:A1:829:CLA:HBB1	1.94	0.48
1:A1:592:TRP:NE1	14:A1:829:CLA:HMD1	2.28	0.48
14:A1:820:CLA:HMD1	14:A1:821:CLA:HBB1	1.96	0.48
1:A2:180:TYR:CE2	14:A2:1613:CLA:C4D	2.97	0.48
1:A3:275:TYR:CZ	14:A3:815:CLA:HMD2	2.48	0.48
1:A3:352:TRP:CZ2	14:A3:825:CLA:H18	2.48	0.48
1:A3:24:SER:O	14:A3:811:CLA:HMA1	2.13	0.48
14:A3:834:CLA:C1	10:L3:62:TRP:NE1	2.76	0.48
1:A4:120:ILE:C	1:A4:122:GLY:H	2.16	0.48
14:A4:820:CLA:CMB	14:A4:824:CLA:HMA3	2.42	0.48
16:A4:847:BCR:H333	16:A4:848:BCR:H333	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:48:ILE:CD1	14:A5:840:CLA:HMA1	2.44	0.48
14:A6:1621:CLA:CMD	14:A6:1622:CLA:HBB1	2.43	0.48
2:B1:723:TYR:CE1	14:B1:804:CLA:CGA	2.96	0.48
2:B1:166:TRP:CZ2	14:B1:814:CLA:HAC2	2.48	0.48
2:B1:463:ALA:N	14:B1:839:CLA:OBD	2.38	0.48
2:B2:303:MET:HA	14:B2:821:CLA:O1D	2.13	0.48
14:B2:813:CLA:HAB	14:B2:827:CLA:H13	1.95	0.48
1:A3:677:LEU:HD11	2:B3:623:MET:HB2	1.94	0.48
2:B4:275:HIS:O	2:B4:279:ILE:HG12	2.13	0.48
2:B4:181:LEU:HD11	14:B4:815:CLA:C1	2.42	0.48
2:B6:589:MET:O	2:B6:593:ILE:HG12	2.12	0.48
14:B6:809:CLA:HMB3	14:B6:810:CLA:CHC	2.43	0.48
3:C5:13:CYS:HB2	3:C5:15:GLN:HE21	1.78	0.48
14:B6:809:CLA:H201	7:I6:23:PRO:CA	2.42	0.48
10:L4:93:LEU:HB3	10:L4:121:THR:HG23	1.94	0.48
1:A4:473:ASP:OD1	10:L4:69:ARG:NH2	2.46	0.48
10:L6:21:ILE:HG21	14:L6:202:CLA:C3D	2.43	0.48
13:P2:27:ASP:OD1	13:P2:41:ARG:NH2	2.46	0.48
1:A2:363:MET:HE3	14:A2:1631:CLA:HMC1	1.95	0.48
14:A3:826:CLA:H162	16:A3:850:BCR:H272	1.95	0.48
1:A4:456:PHE:HE2	14:B4:805:CLA:H92	1.75	0.48
1:A4:604:ASN:HD21	14:A4:801:CLA:H201	1.77	0.48
1:A5:681:PHE:CG	16:A5:850:BCR:H363	2.49	0.48
14:A5:814:CLA:HBA2	14:A5:816:CLA:HMB3	1.94	0.48
1:A5:336:PHE:CB	17:A5:852:LHG:HC41	2.42	0.48
14:B1:815:CLA:HAB	14:B1:829:CLA:H13	1.96	0.48
14:B2:818:CLA:HMB2	14:B2:823:CLA:HMA3	1.94	0.48
2:B3:514:LEU:HD12	14:B3:1828:CLA:CMC	2.43	0.48
2:B4:711:ALA:HB2	15:B4:844:PQN:C8	2.42	0.48
14:B5:1803:CLA:H72	14:B5:1804:CLA:CED	2.44	0.48
2:B5:267:LEU:HD22	14:B5:1819:CLA:HBA1	1.95	0.48
2:B5:642:ASN:HB2	2:B5:643:PRO:HD2	1.94	0.48
2:B6:419:GLU:CD	2:B6:419:GLU:H	2.16	0.48
2:B6:526:HIS:CD2	14:B6:838:CLA:HED3	2.48	0.48
14:B6:830:CLA:HMB2	14:B6:831:CLA:C2D	2.44	0.48
1:A1:453:PHE:C	14:L1:202:CLA:HBB2	2.33	0.48
10:L4:54:HIS:HA	10:L4:57:PHE:CE2	2.48	0.48
13:P3:27:ASP:OD1	13:P3:41:ARG:NH2	2.46	0.48
1:A1:275:TYR:CE2	14:A1:814:CLA:HMD2	2.48	0.48
1:A4:28:TRP:HZ2	14:A4:803:CLA:H11	1.77	0.48
1:A4:488:GLN:NE2	1:A4:531:LEU:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:677:LEU:HD21	2:B4:626:LEU:HD22	1.96	0.48
1:A6:696:TYR:OH	14:A6:1603:CLA:OBD	2.30	0.48
14:A1:839:CLA:HMA1	2:B1:694:ALA:HB1	1.96	0.48
2:B1:181:LEU:HD11	14:B1:814:CLA:C1	2.40	0.48
2:B5:176:HIS:CG	14:B5:1815:CLA:HMC2	2.48	0.48
2:B5:189:TRP:CA	14:B5:1816:CLA:HBB1	2.43	0.48
1:A5:647:ASN:HB2	2:B5:657:LEU:HD11	1.96	0.48
1:A6:468:PHE:HZ	14:B6:809:CLA:CHC	2.26	0.48
7:I2:10:LEU:N	7:I2:11:PRO:CD	2.77	0.48
10:L1:135:ALA:O	10:L1:139:LEU:HG	2.14	0.48
10:L5:65:LEU:HA	10:L5:69:ARG:HD3	1.96	0.48
10:L6:57:PHE:CD1	10:L6:57:PHE:C	2.86	0.48
10:L6:79:LEU:HD22	10:L6:136:PHE:CD2	2.48	0.48
11:M3:17:LEU:HG	14:M3:1601:CLA:CMB	2.43	0.48
1:A1:215:HIS:HB2	14:A1:813:CLA:C1C	2.43	0.48
1:A1:65:LEU:HD23	1:A1:187:LEU:HD21	1.96	0.48
1:A1:682:ILE:CD1	16:A1:847:BCR:H353	2.43	0.48
1:A2:472:GLN:OE1	1:A2:472:GLN:N	2.47	0.48
1:A2:590:SER:OG	1:A2:593:ASP:OD2	2.32	0.48
1:A3:682:ILE:HD12	16:A3:852:BCR:C35	2.44	0.48
1:A6:215:HIS:HB2	14:A6:1614:CLA:CHC	2.43	0.48
2:B1:466:ILE:CD1	14:B1:838:CLA:CGA	2.92	0.48
2:B1:227:GLY:HA2	14:B1:817:CLA:C4	2.43	0.48
2:B1:353:GLN:HG3	14:B1:826:CLA:O1D	2.12	0.48
14:B2:808:CLA:HMB3	14:B2:809:CLA:CHC	2.44	0.48
14:B3:1832:CLA:HMB2	14:B3:1833:CLA:C2D	2.43	0.48
2:B4:481:LEU:CA	2:B4:489:SER:OG	2.61	0.48
14:B4:803:CLA:H72	14:B4:804:CLA:CED	2.44	0.48
2:B4:195:HIS:CG	14:B4:816:CLA:HBC3	2.49	0.48
2:B5:710:GLN:CG	19:B5:1851:LMG:H111	2.44	0.48
1:A6:578:CYS:SG	18:B6:801:SF4:S4	3.03	0.48
2:B6:589:MET:HA	14:B6:825:CLA:HBC1	1.96	0.48
4:D2:39:PHE:CE1	4:D2:67:LEU:HD11	2.48	0.48
8:J1:28:GLU:HG3	14:J1:101:CLA:C1B	2.44	0.48
8:J5:32:PHE:C	8:J5:34:PRO:HD3	2.33	0.48
10:L1:35:PRO:HG3	14:L1:206:CLA:HED2	1.96	0.48
10:L3:46:ARG:O	10:L3:50:VAL:HG23	2.14	0.48
14:L5:204:CLA:C1B	14:L5:205:CLA:HED1	2.43	0.48
14:M1:1201:CLA:HMB2	16:M1:1202:BCR:HC42	1.96	0.48
13:P6:27:ASP:OD1	13:P6:41:ARG:NH2	2.46	0.48
1:A1:215:HIS:HB2	14:A1:813:CLA:CHC	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:360:LEU:HD21	14:A3:830:CLA:CHC	2.44	0.48
1:A4:497:ALA:N	1:A4:498:PRO:CD	2.76	0.48
14:A4:828:CLA:HBB1	14:A4:828:CLA:HMB1	1.94	0.48
14:A4:829:CLA:H111	17:A4:850:LHG:H202	1.95	0.48
1:A5:120:ILE:C	1:A5:122:GLY:H	2.16	0.48
1:A5:90:MET:HE1	14:A5:808:CLA:HAA2	1.94	0.48
14:A5:821:CLA:HAA2	14:A5:825:CLA:HBB1	1.96	0.48
1:A6:189:TRP:CZ3	14:A6:1613:CLA:HMD3	2.49	0.48
2:B1:261:HIS:HD2	2:B1:263:GLN:H	1.60	0.48
2:B1:334:HIS:CE1	2:B1:395:ILE:HG21	2.49	0.48
14:B1:810:CLA:C1A	14:B1:810:CLA:CGA	2.91	0.48
2:B1:189:TRP:CD2	14:B1:819:CLA:HMD3	2.48	0.48
2:B2:350:LEU:HD13	14:B2:825:CLA:HAA1	1.95	0.48
2:B3:384:PHE:CD2	14:B3:1808:CLA:H112	2.48	0.48
2:B3:195:HIS:CG	14:B3:1816:CLA:HBC3	2.47	0.48
14:B3:1810:CLA:O1A	14:B3:1829:CLA:HBD	2.14	0.48
2:B6:562:ALA:HB2	2:B6:579:TRP:CD1	2.49	0.48
2:B6:716:LEU:O	2:B6:720:SER:OG	2.25	0.48
1:A4:582:GLY:HA3	3:C4:48:VAL:O	2.14	0.48
5:E2:7:VAL:O	5:E2:20:VAL:HA	2.14	0.48
5:E5:8:LYS:HA	5:E5:19:GLU:O	2.12	0.48
6:F3:76:TRP:CZ3	14:F3:202:CLA:HBA2	2.48	0.48
6:F4:76:TRP:CZ2	14:F4:202:CLA:O1A	2.67	0.48
6:F6:76:TRP:HZ2	14:F6:202:CLA:O2D	1.95	0.48
14:B5:1843:CLA:C20	7:I5:27:MET:HE3	2.43	0.48
9:K5:63:THR:O	9:K5:67:HIS:N	2.46	0.48
1:A2:189:TRP:CE2	14:A2:1615:CLA:HAC2	2.48	0.48
1:A2:215:HIS:HB2	14:A2:1616:CLA:CHC	2.44	0.48
1:A2:356:LEU:O	1:A2:360:LEU:HB2	2.14	0.48
1:A4:33:HIS:CG	1:A4:34:PHE:N	2.82	0.48
1:A6:120:ILE:C	1:A6:122:GLY:H	2.16	0.48
14:A6:1602:CLA:HMB3	14:A6:1651:CLA:OBD	2.14	0.48
14:A6:1621:CLA:CMB	14:A6:1625:CLA:HMA3	2.43	0.48
1:A6:283:GLY:O	1:A6:508:THR:O	2.32	0.48
2:B2:526:HIS:CG	14:B2:837:CLA:HED3	2.47	0.48
14:B2:832:CLA:H11	8:J2:29:PHE:CE2	2.49	0.48
2:B3:430:LEU:HD12	14:B3:1802:CLA:HBA2	1.94	0.48
14:B4:831:CLA:H8	19:B4:851:LMG:H242	1.95	0.48
14:B5:1816:CLA:HAB	14:B5:1830:CLA:H13	1.96	0.48
14:B5:1826:CLA:H61	14:B5:1828:CLA:H42	1.96	0.48
2:B6:390:PHE:CD1	2:B6:540:LEU:HD13	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C3:54:GLU:HG2	3:C3:62:LEU:HD13	1.95	0.48
6:F5:73:ILE:O	6:F5:76:TRP:HB3	2.12	0.48
16:J5:105:BCR:HC8	16:J5:105:BCR:H331	1.94	0.48
14:B3:1801:CLA:O1A	14:M3:1601:CLA:HAA2	2.13	0.48
16:A1:846:BCR:H382	16:A1:846:BCR:H23C	1.96	0.48
1:A2:161:THR:HG22	16:A2:1648:BCR:HC32	1.96	0.48
16:A2:1650:BCR:H333	16:A2:1651:BCR:H333	1.95	0.48
1:A2:680:HIS:HD2	14:B2:802:CLA:O1D	1.96	0.48
1:A3:259:GLY:C	1:A3:261:PHE:H	2.17	0.48
1:A3:726:GLN:NE2	17:A3:853:LHG:HC81	2.29	0.48
1:A4:565:LEU:HD11	1:A4:583:ARG:HB3	1.95	0.48
1:A5:572:LEU:HD21	3:C5:52:ARG:NH2	2.28	0.48
1:A6:215:HIS:HB2	14:A6:1614:CLA:C1C	2.44	0.48
16:A6:1646:BCR:H333	16:A6:1647:BCR:H333	1.95	0.48
1:A6:741:ALA:HB2	16:A6:1648:BCR:H323	1.96	0.48
14:B1:804:CLA:H72	14:B1:805:CLA:CED	2.44	0.48
2:B1:136:GLN:NE2	14:B1:815:CLA:HBD	2.29	0.48
2:B1:499:TRP:CZ2	14:B1:836:CLA:HMA2	2.49	0.48
2:B2:445:VAL:HG21	14:B2:832:CLA:HAC2	1.96	0.48
14:B3:1810:CLA:HMB2	14:B3:1810:CLA:H142	1.96	0.48
2:B4:256:PHE:CD1	14:B4:819:CLA:HAB	2.47	0.48
14:B4:821:CLA:HMB2	14:B4:826:CLA:HMA3	1.94	0.48
2:B5:466:ILE:HD12	14:B5:1839:CLA:CGA	2.43	0.48
2:B6:642:ASN:HB2	2:B6:643:PRO:HD2	1.95	0.48
2:B6:599:TYR:CE1	14:B6:837:CLA:HBC2	2.49	0.48
2:B6:90:ILE:HB	2:B6:111:PRO:HB2	1.96	0.48
3:C4:3:THR:HG21	4:D4:136:TYR:CE1	2.49	0.48
10:L2:124:PHE:CZ	16:L2:208:BCR:H292	2.49	0.48
10:L5:90:THR:HA	10:L5:93:LEU:HD12	1.95	0.48
14:M2:1201:CLA:HMB2	16:M2:1202:BCR:HC42	1.96	0.48
14:B2:838:CLA:HBC2	14:X2:1701:CLA:HBC3	1.94	0.48
14:A1:820:CLA:CMB	14:A1:824:CLA:HMA3	2.43	0.48
14:A2:1606:CLA:HMC3	14:A2:1608:CLA:HED2	1.96	0.48
1:A2:446:TRP:CD1	14:A2:1644:CLA:O1A	2.67	0.48
1:A3:283:GLY:O	1:A3:508:THR:O	2.32	0.48
1:A3:686:SER:HB3	1:A3:734:HIS:CB	2.44	0.48
1:A4:399:TRP:NE1	14:A4:827:CLA:HAB	2.29	0.48
1:A5:259:GLY:C	1:A5:261:PHE:H	2.16	0.48
1:A5:34:PHE:CD1	1:A5:61:HIS:CE1	3.02	0.48
1:A6:475:PHE:HA	1:A6:480:ILE:O	2.14	0.48
2:B1:290:TYR:OH	14:B1:820:CLA:O1D	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:50:PHE:CD1	2:B2:152:GLY:HA2	2.49	0.48
2:B2:738:LYS:O	2:B2:739:PHE:CB	2.60	0.48
2:B3:350:LEU:HD23	14:B3:1820:CLA:H62	1.96	0.48
16:B3:1851:BCR:H331	16:B3:1851:BCR:HC8	1.96	0.48
2:B3:231:VAL:O	2:B3:234:GLN:HG2	2.14	0.48
2:B4:188:ALA:CB	14:B4:830:CLA:H202	2.43	0.48
1:A4:651:ARG:HD2	2:B4:639:ASN:ND2	2.29	0.48
14:A4:831:CLA:HMA1	2:B4:691:THR:OG1	2.13	0.48
14:B4:819:CLA:H3A	14:B4:819:CLA:HBA2	1.47	0.48
2:B4:466:ILE:HD13	14:B4:836:CLA:HBB1	1.96	0.48
14:B4:852:CLA:CBA	14:A6:1601:CLA:HAA2	2.43	0.48
2:B5:361:TYR:HE2	14:B5:1820:CLA:O2D	1.97	0.48
2:B5:573:THR:O	2:B5:576:ILE:HB	2.14	0.48
14:B6:807:CLA:H61	14:B6:807:CLA:H41	1.69	0.48
4:D2:30:THR:O	4:D2:80:TYR:HA	2.14	0.48
5:E6:68:VAL:O	5:E6:69:ALA:O	2.31	0.48
6:F1:73:ILE:HG23	14:F1:1301:CLA:HAA1	1.96	0.48
6:F4:63:PHE:C	6:F4:66:PRO:HD2	2.35	0.48
8:J4:33:TYR:N	8:J4:34:PRO:HD3	2.29	0.48
10:L4:134:VAL:CB	16:L4:208:BCR:H403	2.44	0.48
17:B6:849:LHG:HC2	12:X6:12:ARG:NH2	2.29	0.48
14:A4:830:CLA:HBB1	14:A4:837:CLA:CBB	2.44	0.47
1:A5:215:HIS:HB2	14:A5:814:CLA:C1C	2.44	0.47
14:A6:1604:CLA:HMC3	14:A6:1606:CLA:HED2	1.96	0.47
2:B1:288:HIS:O	14:B1:822:CLA:HHD	2.14	0.47
2:B2:90:ILE:HB	2:B2:111:PRO:HB2	1.93	0.47
2:B3:664:ALA:HB3	14:B3:1805:CLA:HBB2	1.95	0.47
2:B4:157:GLN:O	2:B4:161:ARG:HG3	2.14	0.47
2:B4:28:HIS:CE1	14:B4:808:CLA:HED1	2.49	0.47
2:B4:229:TRP:CD2	14:B4:818:CLA:HMB2	2.49	0.47
14:B4:826:CLA:H61	14:B4:828:CLA:H42	1.96	0.47
14:B5:1827:CLA:HBA2	14:B5:1827:CLA:H3A	1.73	0.47
2:B6:286:ALA:HB2	14:B6:819:CLA:HBC2	1.95	0.47
3:C5:17:VAL:HG22	3:C5:25:LEU:HB2	1.96	0.47
6:F2:77:ILE:HG12	14:F2:202:CLA:C4D	2.44	0.47
14:B1:811:CLA:C20	7:I1:26:VAL:CG2	2.85	0.47
7:I1:30:LEU:HD13	16:I1:103:BCR:C7	2.44	0.47
9:K3:74:VAL:C	9:K3:76:GLY:H	2.16	0.47
9:K4:74:VAL:C	9:K4:76:GLY:H	2.17	0.47
10:L2:41:LEU:HD13	10:L2:45:LEU:HD23	1.96	0.47
10:L3:115:GLU:N	10:L3:115:GLU:OE1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B4:806:CLA:H3A	11:M4:29:LEU:HD13	1.96	0.47
13:P5:27:ASP:OD1	13:P5:41:ARG:NH2	2.46	0.47
2:B5:462:PHE:CE2	14:X5:101:CLA:HBD	2.48	0.47
1:A2:272:TRP:HZ3	14:A2:1619:CLA:H2	1.79	0.47
1:A3:444:LEU:HD11	1:A3:547:HIS:HD2	1.78	0.47
1:A4:297:THR:O	1:A4:300:HIS:HB3	2.14	0.47
1:A4:283:GLY:O	1:A4:508:THR:O	2.31	0.47
1:A4:56:HIS:HB3	14:A4:804:CLA:HAB	1.95	0.47
1:A5:283:GLY:O	1:A5:508:THR:O	2.31	0.47
16:A5:848:BCR:H333	16:A5:849:BCR:H333	1.95	0.47
2:B1:531:LEU:HD21	14:B1:805:CLA:CBB	2.44	0.47
2:B1:430:LEU:HD13	14:B1:802:CLA:HED3	1.95	0.47
2:B4:125:THR:HG22	14:B4:820:CLA:HED1	1.95	0.47
2:B4:430:LEU:HD11	16:F4:201:BCR:C40	2.44	0.47
2:B4:532:GLY:HA2	2:B4:588:TRP:CZ3	2.48	0.47
2:B6:725:LEU:HD11	14:B6:829:CLA:H203	1.96	0.47
6:F1:61:GLY:HA3	8:J1:39:HIS:O	2.15	0.47
14:B4:833:CLA:HBC3	16:F4:203:BCR:H362	1.96	0.47
7:I1:16:PRO:HB3	7:I1:20:TRP:CE3	2.48	0.47
2:B3:91:TRP:CZ3	7:I3:1:MET:HB3	2.50	0.47
8:J2:24:GLY:HA3	14:J2:101:CLA:CBB	2.38	0.47
12:X3:12:ARG:HB3	17:X3:101:LHG:C4	2.44	0.47
12:X4:23:ASN:OD1	14:X4:102:CLA:NA	2.47	0.47
14:A1:813:CLA:HBA2	14:A1:815:CLA:HMB3	1.95	0.47
14:A2:1606:CLA:H2	14:A2:1613:CLA:H92	1.96	0.47
16:A3:852:BCR:H362	14:B3:1804:CLA:C4	2.35	0.47
14:A4:809:CLA:HBA2	14:A4:809:CLA:H3A	1.71	0.47
14:A4:825:CLA:H162	16:A4:847:BCR:H272	1.96	0.47
1:A5:375:TYR:CE1	1:A5:376:ALA:HB2	2.48	0.47
1:A5:587:CYS:HB2	2:B5:673:TRP:HB3	1.95	0.47
1:A5:744:TRP:CD2	16:A5:850:BCR:HC22	2.49	0.47
1:A6:302:LEU:HD21	14:A6:1617:CLA:C3B	2.45	0.47
2:B1:290:TYR:CE2	14:B1:820:CLA:O1D	2.68	0.47
1:A1:470:ARG:NH1	2:B1:94:GLN:O	2.46	0.47
2:B2:717:ALA:HA	19:B2:848:LMG:H371	1.97	0.47
2:B3:622:LEU:HD11	14:B3:1803:CLA:H202	1.96	0.47
14:L4:205:CLA:HMD1	14:B5:1812:CLA:H203	1.97	0.47
14:B6:810:CLA:CGA	10:L5:148:ILE:HG12	2.44	0.47
14:B6:835:CLA:HBA2	14:B6:836:CLA:HMB3	1.97	0.47
4:D6:30:THR:O	4:D6:80:TYR:HA	2.13	0.47
10:L1:110:PRO:O	10:L1:113:THR:OG1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D2:17:LEU:HG	10:L2:13:PHE:O	2.14	0.47
1:A2:40:ARG:HG3	13:P2:60:SER:CB	2.44	0.47
1:A2:283:GLY:O	1:A2:508:THR:O	2.32	0.47
1:A2:539:HIS:CG	14:A2:1639:CLA:HED2	2.49	0.47
1:A3:459:TYR:OH	1:A3:538:VAL:HG13	2.14	0.47
14:A3:831:CLA:HBB1	14:A3:839:CLA:CBB	2.45	0.47
1:A4:47:TRP:CZ3	1:A4:51:LEU:HD12	2.49	0.47
1:A4:353:HIS:CD2	14:A4:804:CLA:HBC1	2.48	0.47
1:A5:204:LEU:HD11	14:A5:829:CLA:C14	2.44	0.47
1:A5:257:ASP:OD1	1:A5:258:TRP:N	2.46	0.47
1:A5:332:HIS:CD2	14:A5:843:CLA:CMC	2.97	0.47
2:B1:573:THR:O	2:B1:576:ILE:HB	2.14	0.47
16:B1:852:BCR:HC8	16:B1:852:BCR:H331	1.95	0.47
2:B3:493:PRO:CG	14:B3:1838:CLA:C4D	2.90	0.47
2:B3:470:HIS:HA	14:B3:1836:CLA:HED3	1.96	0.47
2:B3:669:PHE:HA	15:B3:1844:PQN:O1	2.14	0.47
2:B4:592:THR:O	2:B4:596:VAL:HG13	2.14	0.47
2:B4:652:TRP:CH2	14:B4:810:CLA:CBC	2.97	0.47
2:B6:380:TYR:CD1	2:B6:593:ILE:HG21	2.49	0.47
14:B6:803:CLA:C19	6:F6:84:TYR:HB2	2.45	0.47
2:B6:52:HIS:CE1	14:B6:806:CLA:HMA1	2.48	0.47
2:B6:8:SER:HA	2:B6:34:ASP:OD2	2.14	0.47
3:C4:14:THR:HG22	3:C4:27:MET:HG3	1.96	0.47
8:J4:21:ILE:HA	14:J4:101:CLA:HBB2	1.96	0.47
10:L6:21:ILE:HG21	14:L6:202:CLA:C4D	2.44	0.47
14:A2:1631:CLA:HBB1	14:A2:1631:CLA:HMB1	1.95	0.47
14:A4:821:CLA:H3A	14:A4:821:CLA:HBA2	1.52	0.47
1:A5:387:TYR:CE2	1:A5:622:TRP:CD1	3.03	0.47
14:A5:829:CLA:HBB1	14:A5:829:CLA:HMB1	1.96	0.47
16:A5:849:BCR:H23C	16:A5:849:BCR:H382	1.96	0.47
14:A6:1626:CLA:H162	16:A6:1646:BCR:H272	1.97	0.47
1:A6:56:HIS:CG	14:A6:1605:CLA:HAB	2.50	0.47
2:B1:398:VAL:HG23	2:B1:547:ALA:HB1	1.97	0.47
2:B1:358:LEU:HG	14:B1:827:CLA:HMC2	1.96	0.47
14:B2:808:CLA:H102	14:B2:826:CLA:H193	1.96	0.47
14:B3:1810:CLA:C1A	14:B3:1810:CLA:CGA	2.93	0.47
14:B3:1827:CLA:H3A	14:B3:1827:CLA:HBA2	1.75	0.47
14:B3:1816:CLA:HAB	14:B3:1830:CLA:H13	1.96	0.47
2:B3:537:THR:HG21	14:B3:1827:CLA:HBB2	1.96	0.47
2:B4:173:ARG:HB2	14:B4:815:CLA:HBC2	1.96	0.47
2:B4:361:TYR:O	2:B4:364:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:466:ARG:HG2	2:B5:641:TYR:HD1	1.79	0.47
3:C2:13:CYS:O	3:C2:15:GLN:NE2	2.47	0.47
1:A4:572:LEU:HD21	3:C4:52:ARG:NH2	2.30	0.47
6:F6:99:ILE:O	8:J6:11:ALA:N	2.43	0.47
7:I3:20:TRP:CE2	16:I3:102:BCR:HC22	2.49	0.47
7:I4:9:PHE:CE1	7:I4:10:LEU:HD13	2.49	0.47
7:I6:23:PRO:HA	7:I6:26:VAL:HG22	1.96	0.47
10:L4:53:ALA:HB2	14:L4:204:CLA:HED3	1.97	0.47
14:A1:816:CLA:ND	14:A1:816:CLA:H11	2.29	0.47
1:A2:215:HIS:HB2	14:A2:1616:CLA:C1C	2.45	0.47
1:A2:360:LEU:HD13	14:A2:1632:CLA:HBB1	1.97	0.47
1:A2:403:PHE:HB3	14:A2:1608:CLA:H112	1.97	0.47
14:A3:822:CLA:H3A	14:A3:822:CLA:HBA2	1.51	0.47
1:A6:377:MET:N	1:A6:378:PRO:CD	2.78	0.47
2:B1:442:HIS:HE1	14:B1:834:CLA:C4D	2.28	0.47
2:B1:727:TYR:N	14:B1:804:CLA:O1D	2.46	0.47
2:B1:53:LEU:HD13	14:B1:807:CLA:CGA	2.42	0.47
14:B1:810:CLA:H142	14:B1:810:CLA:HMB2	1.97	0.47
14:B1:811:CLA:HMB3	14:B1:854:CLA:CHC	2.45	0.47
2:B1:173:ARG:NE	14:B1:825:CLA:HMD1	2.30	0.47
14:B1:825:CLA:H61	14:B1:827:CLA:H42	1.97	0.47
2:B2:637:LEU:HD21	2:B2:656:PHE:CD1	2.49	0.47
14:B2:830:CLA:HBC3	16:F2:203:BCR:H362	1.97	0.47
14:B3:1808:CLA:H41	14:B3:1808:CLA:H61	1.69	0.47
14:B3:1811:CLA:HMB3	14:B3:1812:CLA:CHC	2.45	0.47
2:B3:184:VAL:HG12	16:B3:1846:BCR:H352	1.95	0.47
2:B4:7:PHE:CD1	2:B4:33:HIS:CD2	3.01	0.47
2:B4:438:GLY:HA3	14:B4:835:CLA:HBB1	1.97	0.47
2:B4:229:TRP:HB2	14:B4:818:CLA:H12	1.95	0.47
14:B5:1830:CLA:HBA2	14:B5:1830:CLA:H3A	1.71	0.47
2:B5:261:HIS:HD2	2:B5:263:GLN:N	2.11	0.47
14:L2:205:CLA:H43	14:L2:205:CLA:HMB2	1.97	0.47
10:L6:35:PRO:HD2	14:L6:207:CLA:OBD	2.14	0.47
1:A1:118:TRP:HB3	16:J1:104:BCR:HC21	1.97	0.47
1:A1:28:TRP:HZ2	14:A1:803:CLA:H11	1.78	0.47
1:A1:74:SER:OG	1:A1:180:TYR:HB2	2.15	0.47
1:A2:352:TRP:CZ3	14:A2:1627:CLA:H112	2.49	0.47
14:A2:1633:CLA:HBB1	14:A2:1640:CLA:CBB	2.45	0.47
1:A3:120:ILE:C	1:A3:122:GLY:H	2.16	0.47
14:A3:804:CLA:HMC3	14:A3:806:CLA:HED2	1.97	0.47
14:A3:821:CLA:CMB	14:A3:825:CLA:HMA3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A3:829:CLA:HMB1	14:A3:829:CLA:HBB1	1.95	0.47
1:A4:549:THR:OG1	1:A4:601:TRP:HB3	2.14	0.47
14:A4:816:CLA:H11	14:A4:816:CLA:ND	2.29	0.47
1:A5:297:THR:O	1:A5:300:HIS:HB3	2.15	0.47
1:A5:40:ARG:HD3	13:P5:61:ASP:CA	2.36	0.47
14:A5:817:CLA:ND	14:A5:817:CLA:H11	2.29	0.47
2:B1:622:LEU:HD13	14:B1:805:CLA:HMA2	1.97	0.47
2:B2:59:TRP:CD1	14:B2:805:CLA:HBC1	2.49	0.47
2:B2:357:SER:HB2	14:B2:825:CLA:HMC1	1.97	0.47
14:A3:801:CLA:HMB3	14:B3:1804:CLA:OBD	2.15	0.47
2:B3:377:HIS:O	2:B3:381:ILE:HG12	2.14	0.47
2:B3:720:SER:O	2:B3:724:ILE:HD12	2.15	0.47
2:B4:573:THR:O	2:B4:576:ILE:HB	2.14	0.47
2:B4:693:LEU:HD21	10:L4:34:LEU:HD23	1.97	0.47
2:B4:724:ILE:HD13	14:B4:829:CLA:HMC2	1.97	0.47
14:B4:810:CLA:H142	14:B4:810:CLA:HMB2	1.96	0.47
14:B5:1810:CLA:H142	14:B5:1810:CLA:HMB2	1.97	0.47
2:B6:26:MET:SD	19:B6:848:LMG:HC1	2.54	0.47
2:B6:599:TYR:CE2	14:B6:837:CLA:C3C	2.98	0.47
2:B6:688:HIS:HE1	2:B6:697:VAL:O	1.96	0.47
1:A6:582:GLY:HA3	3:C6:48:VAL:O	2.14	0.47
6:F3:103:VAL:HB	6:F3:104:PRO:HD3	1.95	0.47
6:F5:55:GLY:O	6:F5:56:ARG:C	2.52	0.47
8:J5:13:VAL:HG22	16:J5:104:BCR:H292	1.96	0.47
1:A1:13:ARG:O	14:A1:811:CLA:HED3	2.15	0.47
14:A1:821:CLA:H3A	14:A1:821:CLA:HBA2	1.52	0.47
1:A1:161:THR:HG22	16:A1:843:BCR:HC32	1.97	0.47
14:A1:825:CLA:H162	16:A1:845:BCR:H272	1.96	0.47
14:A2:1623:CLA:HMD1	14:A2:1624:CLA:HBB1	1.96	0.47
1:A3:244:LEU:C	1:A3:246:PRO:HD3	2.35	0.47
14:A3:804:CLA:H2	14:A3:811:CLA:H92	1.96	0.47
14:A3:809:CLA:HBC2	14:A3:828:CLA:H141	1.95	0.47
14:A6:1631:CLA:HBB1	14:A6:1638:CLA:CBB	2.45	0.47
1:A6:464:THR:HG22	1:A6:468:PHE:HE1	1.79	0.47
2:B1:642:ASN:HB2	2:B1:643:PRO:HD2	1.96	0.47
2:B1:339:TRP:CE2	14:B1:827:CLA:H91	2.49	0.47
1:A2:706:TRP:CG	2:B2:419:GLU:HG3	2.49	0.47
2:B3:188:ALA:HA	14:B3:1817:CLA:HBB2	1.96	0.47
14:B3:1837:CLA:HBA2	14:B3:1838:CLA:HMB3	1.97	0.47
2:B5:188:ALA:HA	14:B5:1817:CLA:HBB2	1.95	0.47
2:B5:318:PHE:CD1	14:B5:1824:CLA:HAB	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B6:343:CYS:HA	14:B6:826:CLA:H51	1.96	0.47
14:B6:803:CLA:H191	6:F6:84:TYR:HB2	1.97	0.47
4:D2:50:ARG:H	4:D2:54:ASN:HD21	1.63	0.47
6:F2:69:LEU:CB	14:F2:204:CLA:HBB2	2.45	0.47
6:F6:70:PHE:HD1	16:F6:201:BCR:H321	1.80	0.47
10:L2:65:LEU:HB3	14:L2:202:CLA:HMA2	1.95	0.47
14:B4:812:CLA:H162	10:L6:56:TYR:OH	2.14	0.47
14:A1:820:CLA:HAA2	14:A1:824:CLA:HBB1	1.96	0.47
16:A1:845:BCR:H333	16:A1:846:BCR:H333	1.96	0.47
14:A2:1619:CLA:H11	14:A2:1619:CLA:ND	2.30	0.47
14:A2:1632:CLA:H111	17:A2:1653:LHG:H202	1.95	0.47
16:A3:851:BCR:H23C	16:A3:851:BCR:H382	1.97	0.47
14:A4:801:CLA:HAA2	14:A4:801:CLA:CGD	2.45	0.47
1:A5:221:LEU:HD11	1:A5:295:SER:HB3	1.97	0.47
14:A5:821:CLA:HMD1	14:A5:822:CLA:HBB1	1.97	0.47
14:A6:1619:CLA:O1A	14:A6:1629:CLA:HMD1	2.15	0.47
1:A6:297:THR:O	1:A6:300:HIS:HB3	2.15	0.47
1:A6:465:MET:SD	1:A6:470:ARG:CZ	3.03	0.47
1:A6:473:ASP:HA	10:L6:69:ARG:NH2	2.28	0.47
14:B2:801:CLA:H72	14:B2:802:CLA:CED	2.45	0.47
2:B2:65:PHE:CE2	14:B2:806:CLA:CHD	2.97	0.47
14:B2:808:CLA:H201	7:I2:23:PRO:CA	2.45	0.47
2:B2:181:LEU:HD11	14:B2:812:CLA:H43	1.97	0.47
2:B4:706:LEU:HG	15:B4:844:PQN:O4	2.14	0.47
2:B5:122:TRP:HB2	2:B5:361:TYR:CE1	2.49	0.47
2:B5:521:GLY:O	2:B5:525:VAL:HG22	2.15	0.47
4:D1:30:THR:O	4:D1:80:TYR:HA	2.13	0.47
4:D2:17:LEU:O	10:L2:15:GLY:N	2.36	0.47
9:K2:74:VAL:C	9:K2:76:GLY:H	2.18	0.47
1:A1:40:ARG:HG3	13:P1:61:ASP:HA	1.95	0.47
1:A1:99:ASN:HB3	1:A1:134:PHE:CG	2.50	0.47
1:A1:565:LEU:HD11	1:A1:583:ARG:HB3	1.96	0.47
1:A2:744:TRP:HB2	14:A2:1630:CLA:HBB1	1.97	0.47
1:A2:546:ILE:O	1:A2:550:VAL:HG23	2.14	0.47
16:A3:850:BCR:H333	16:A3:851:BCR:H333	1.95	0.47
1:A4:86:TRP:O	1:A4:90:MET:HG2	2.15	0.47
1:A5:475:PHE:HA	1:A5:480:ILE:O	2.15	0.47
1:A5:683:TRP:NE1	14:A5:801:CLA:HBA2	2.29	0.47
2:B1:625:TRP:O	2:B1:629:TYR:HB3	2.15	0.47
2:B1:144:LEU:HD21	14:B1:815:CLA:H152	1.96	0.47
2:B2:564:PRO:O	2:B2:565:CYS:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:272:MET:HG2	14:B3:1820:CLA:HMA3	1.97	0.47
2:B3:440:TYR:CE1	2:B3:524:LEU:HB3	2.50	0.47
2:B4:442:HIS:CD2	2:B4:456:ILE:HD12	2.50	0.47
14:B4:820:CLA:H41	14:B4:820:CLA:H62	1.78	0.47
2:B5:173:ARG:HB2	14:B5:1815:CLA:HBC2	1.96	0.47
14:A5:841:CLA:CMC	14:B5:1802:CLA:H71	2.43	0.47
14:B5:1825:CLA:CBB	14:B5:1832:CLA:HMD2	2.44	0.47
2:B6:717:ALA:HA	19:B6:848:LMG:H371	1.97	0.47
4:D3:129:LYS:HE2	4:D3:130:PHE:CE1	2.50	0.47
4:D4:30:THR:O	4:D4:80:TYR:HA	2.14	0.47
4:D6:117:ARG:CG	4:D6:121:GLN:HB2	2.45	0.47
9:K1:73:VAL:CB	14:K1:1401:CLA:HBB1	2.44	0.47
1:A1:283:GLY:O	1:A1:508:THR:O	2.32	0.47
14:A2:1628:CLA:H162	16:A2:1650:BCR:H272	1.96	0.47
1:A3:215:HIS:HB2	14:A3:814:CLA:CHC	2.45	0.47
1:A3:391:LEU:O	1:A3:395:THR:HG23	2.15	0.47
1:A3:352:TRP:HB3	14:A3:805:CLA:HAC1	1.97	0.47
1:A4:572:LEU:HD21	3:C4:52:ARG:CZ	2.45	0.47
1:A4:688:MET:O	1:A4:692:SER:OG	2.28	0.47
1:A5:189:TRP:CZ2	14:A5:813:CLA:HAC2	2.49	0.47
14:A5:809:CLA:HBC2	14:A5:828:CLA:H141	1.96	0.47
14:A6:1610:CLA:H3A	14:A6:1610:CLA:HBA2	1.71	0.47
2:B1:547:ALA:O	2:B1:556:LYS:HD2	2.15	0.47
2:B1:668:MET:HE2	14:B1:806:CLA:NB	2.29	0.47
2:B2:49:HIS:HE1	14:B2:804:CLA:H162	1.80	0.47
14:B3:1803:CLA:H72	14:B3:1804:CLA:CED	2.45	0.47
14:B3:1806:CLA:H2	11:M3:26:SER:OG	2.14	0.47
2:B4:117:SER:HA	14:B4:829:CLA:HMA2	1.97	0.47
2:B5:373:ALA:HB1	14:B5:1829:CLA:HMA1	1.97	0.47
2:B6:661:LEU:HD13	14:B6:802:CLA:HAA1	1.97	0.47
14:B6:817:CLA:H3A	14:B6:817:CLA:HBA2	1.44	0.47
14:B1:809:CLA:HMD1	7:I1:10:LEU:HD23	1.97	0.47
7:I5:23:PRO:O	7:I5:24:THR:C	2.53	0.47
8:J3:31:ARG:NH1	14:J3:101:CLA:HED2	2.30	0.47
11:M3:23:PHE:O	11:M3:27:THR:HG23	2.15	0.47
14:M6:1201:CLA:HMB2	16:M6:1202:BCR:HC42	1.97	0.47
1:A1:56:HIS:HB3	14:A1:804:CLA:HAB	1.97	0.46
1:A1:681:PHE:CD2	16:A1:847:BCR:H363	2.50	0.46
14:A1:820:CLA:CMD	14:A1:821:CLA:HBB1	2.45	0.46
14:A1:826:CLA:HBB1	14:A1:832:CLA:HMA2	1.97	0.46
1:A2:79:HIS:CE1	14:A2:1607:CLA:HMA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A2:1644:CLA:H41	14:A2:1644:CLA:H62	1.68	0.46
1:A2:189:TRP:CH2	14:A2:1615:CLA:HHD	2.50	0.46
14:A6:1617:CLA:ND	14:A6:1617:CLA:H11	2.29	0.46
14:A6:1635:CLA:HBA2	14:A6:1635:CLA:H3A	1.76	0.46
1:A6:359:ASN:N	1:A6:359:ASN:ND2	2.63	0.46
2:B2:150:PHE:HD2	14:B2:810:CLA:HBC2	1.78	0.46
14:B2:834:CLA:HBA2	14:B2:835:CLA:HMB3	1.97	0.46
2:B2:288:HIS:NE2	16:B2:842:BCR:H363	2.30	0.46
2:B3:481:LEU:HD12	14:B3:1836:CLA:HED3	1.96	0.46
2:B3:398:VAL:HG23	2:B3:547:ALA:HB1	1.96	0.46
2:B4:313:LYS:O	2:B4:314:VAL:CG2	2.60	0.46
2:B4:564:PRO:O	2:B4:565:CYS:HB3	2.15	0.46
2:B4:339:TRP:HE1	14:B4:826:CLA:C3B	2.28	0.46
2:B5:119:VAL:HB	2:B5:123:TRP:CH2	2.49	0.46
2:B5:122:TRP:HZ2	14:B5:1815:CLA:H191	1.78	0.46
2:B5:514:LEU:HD12	14:B5:1828:CLA:CMC	2.44	0.46
2:B5:654:TRP:CD2	14:B5:1811:CLA:HMC2	2.50	0.46
2:B6:428:VAL:HG12	2:B6:432:LEU:HD12	1.96	0.46
2:B6:456:ILE:HG22	2:B6:458:ILE:CD1	2.45	0.46
1:A6:578:CYS:HG	18:B6:801:SF4:FE3	1.30	0.46
14:B6:808:CLA:H142	14:B6:808:CLA:HMB2	1.97	0.46
14:B6:831:CLA:HBC3	16:F6:203:BCR:H362	1.96	0.46
14:B6:835:CLA:HMB1	16:B6:847:BCR:HC31	1.98	0.46
3:C2:14:THR:HG22	3:C2:27:MET:HG3	1.97	0.46
4:D3:30:THR:O	4:D3:80:TYR:HA	2.15	0.46
16:L2:201:BCR:H272	16:L3:201:BCR:H282	1.97	0.46
10:L3:52:MET:SD	14:L3:203:CLA:HED2	2.55	0.46
10:L5:117:TRP:O	10:L5:120:PHE:HB3	2.16	0.46
14:B4:806:CLA:HMB2	16:M4:101:BCR:HC42	1.97	0.46
1:A3:647:ASN:HB2	2:B3:641:TYR:OH	2.15	0.46
1:A3:655:TRP:CD1	2:B3:631:TRP:CD1	3.04	0.46
1:A4:475:PHE:HA	1:A4:480:ILE:O	2.15	0.46
1:A4:543:ALA:HB1	14:A4:836:CLA:HMB3	1.96	0.46
1:A5:16:VAL:HG11	1:A5:183:ARG:HB3	1.97	0.46
1:A5:244:LEU:C	1:A5:246:PRO:HD3	2.36	0.46
1:A5:444:LEU:HB2	14:A5:838:CLA:CBB	2.45	0.46
1:A6:744:TRP:HB2	14:A6:1628:CLA:HBB1	1.96	0.46
2:B1:456:ILE:HG22	2:B1:458:ILE:HD11	1.97	0.46
14:A1:837:CLA:HMD1	14:B1:803:CLA:HBB1	1.98	0.46
2:B1:50:PHE:CE2	14:B1:814:CLA:HED1	2.50	0.46
2:B2:642:ASN:HB2	2:B2:643:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B2:823:CLA:H61	14:B2:825:CLA:H42	1.97	0.46
14:B3:1818:CLA:HBA2	14:B3:1818:CLA:H3A	1.74	0.46
2:B3:392:HIS:HE1	14:B3:1831:CLA:NA	2.11	0.46
2:B4:433:GLY:HA2	2:B4:531:LEU:HD22	1.96	0.46
2:B5:59:TRP:HA	14:B5:1809:CLA:HBB2	1.97	0.46
14:B5:1811:CLA:H102	14:B5:1829:CLA:H193	1.97	0.46
14:B5:1832:CLA:HBA2	14:B5:1832:CLA:H3A	1.56	0.46
2:B5:577:SER:HG	2:B5:577:SER:H	1.56	0.46
1:A4:422:PRO:HG3	4:D4:40:GLU:HB2	1.96	0.46
6:F2:103:VAL:HB	6:F2:104:PRO:HD3	1.97	0.46
7:I4:13:ILE:C	7:I4:16:PRO:HD2	2.35	0.46
9:K1:74:VAL:C	9:K1:76:GLY:H	2.18	0.46
10:L1:54:HIS:HA	10:L1:57:PHE:CE2	2.50	0.46
14:L1:205:CLA:OBD	10:L3:91:ALA:HA	2.15	0.46
10:L5:37:TYR:O	10:L5:38:ARG:C	2.53	0.46
5:E6:39:ARG:NH1	13:P6:24:TYR:CZ	2.83	0.46
1:A2:557:VAL:HG11	14:A2:1623:CLA:C20	2.45	0.46
1:A2:548:VAL:HG11	1:A2:601:TRP:CZ2	2.51	0.46
1:A3:691:PHE:N	1:A3:691:PHE:CD1	2.83	0.46
1:A4:270:PHE:CD1	14:A4:842:CLA:HMD2	2.50	0.46
1:A5:689:PHE:CE2	1:A5:730:VAL:HG11	2.50	0.46
14:A5:839:CLA:HBB1	14:A5:840:CLA:HMD1	1.96	0.46
14:A5:842:CLA:H62	14:A5:842:CLA:H41	1.68	0.46
1:A6:313:HIS:NE2	16:A6:1643:BCR:H363	2.30	0.46
1:A6:544:PHE:HZ	14:B6:802:CLA:HBB2	1.78	0.46
2:B1:144:LEU:CD2	14:B1:815:CLA:H152	2.45	0.46
2:B1:229:TRP:CG	14:B1:817:CLA:H12	2.50	0.46
2:B1:499:TRP:HZ2	14:B1:836:CLA:CMA	2.29	0.46
2:B1:189:TRP:HA	14:B1:815:CLA:HBB1	1.98	0.46
2:B2:428:VAL:HG21	14:B2:838:CLA:C2C	2.45	0.46
2:B2:651:VAL:HG11	14:B2:808:CLA:HMD2	1.96	0.46
14:B2:837:CLA:HMB2	14:B2:838:CLA:C2D	2.45	0.46
14:B2:834:CLA:HMB1	16:B2:846:BCR:HC31	1.97	0.46
2:B3:677:TRP:HH2	14:B3:1805:CLA:C3D	2.28	0.46
14:B3:1830:CLA:HBA2	14:B3:1830:CLA:H3A	1.71	0.46
2:B3:678:GLN:NE2	2:B3:705:ALA:H	2.13	0.46
2:B4:535:THR:HB	2:B4:588:TRP:CZ3	2.50	0.46
2:B4:7:PHE:HB2	2:B4:33:HIS:CG	2.50	0.46
14:B5:1810:CLA:CGA	14:B5:1810:CLA:C1A	2.93	0.46
14:B5:1843:CLA:H202	7:I5:27:MET:HE3	1.96	0.46
2:B6:600:TRP:HB2	14:B6:837:CLA:HMC1	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B6:599:TYR:CD2	14:B6:837:CLA:HMC2	2.51	0.46
3:C1:24:VAL:O	3:C1:42:PRO:HD2	2.15	0.46
4:D3:117:ARG:NH2	4:D3:138:PRO:OXT	2.47	0.46
4:D4:39:PHE:CE2	4:D4:47:ALA:HB3	2.51	0.46
5:E6:7:VAL:O	5:E6:20:VAL:HA	2.15	0.46
14:L4:203:CLA:H43	14:L4:203:CLA:HMB2	1.97	0.46
10:L6:59:ILE:HD11	10:L6:135:ALA:HB1	1.97	0.46
1:A1:257:ASP:OD1	1:A1:258:TRP:N	2.48	0.46
14:A1:808:CLA:HBC2	14:A1:827:CLA:H141	1.97	0.46
1:A2:544:PHE:CZ	14:A2:1603:CLA:CBB	2.99	0.46
1:A2:244:LEU:C	1:A2:246:PRO:HD3	2.35	0.46
1:A5:436:HIS:HA	4:D5:14:THR:HG23	1.98	0.46
14:A5:826:CLA:H162	16:A5:848:BCR:H272	1.96	0.46
1:A6:447:VAL:HG21	14:A6:1638:CLA:HMC3	1.97	0.46
2:B1:7:PHE:CD1	2:B1:33:HIS:CD2	3.02	0.46
2:B1:600:TRP:CD1	14:B1:838:CLA:HAC1	2.51	0.46
2:B1:665:THR:N	14:B1:806:CLA:HBB1	2.30	0.46
14:B2:827:CLA:H12	16:B2:843:BCR:H393	1.98	0.46
14:B3:1840:CLA:HMB2	14:B3:1841:CLA:C2D	2.46	0.46
2:B3:719:PHE:C	2:B3:719:PHE:CD2	2.87	0.46
1:A4:466:ARG:O	2:B4:646:THR:CG2	2.63	0.46
14:B6:814:CLA:HAB	14:B6:828:CLA:H13	1.97	0.46
14:B6:823:CLA:CBB	14:B6:830:CLA:HMD2	2.45	0.46
3:C5:20:CYS:SG	18:C5:101:SF4:S4	3.13	0.46
4:D6:101:PHE:HB3	4:D6:103:GLU:OE2	2.16	0.46
6:F1:88:VAL:HG11	6:F1:97:LYS:CB	2.43	0.46
7:I1:7:ALA:N	11:M1:5:ASP:OD1	2.46	0.46
6:F3:40:GLN:OE1	8:J3:40:PRO:O	2.33	0.46
14:L1:207:CLA:C9	14:B3:1812:CLA:H101	2.45	0.46
10:L1:58:LEU:CD1	10:L1:85:LEU:HD12	2.45	0.46
14:B1:854:CLA:H141	10:L2:56:TYR:HE1	1.81	0.46
7:I4:37:GLU:N	10:L4:102:GLN:OE1	2.48	0.46
1:A1:615:TRP:HB2	1:A1:653:PHE:CE1	2.51	0.46
14:A1:825:CLA:HAB	16:A1:846:BCR:H311	1.98	0.46
14:A1:839:CLA:H52	14:I1:101:CLA:H43	1.98	0.46
14:A3:821:CLA:CMD	14:A3:822:CLA:HBB1	2.45	0.46
14:A4:803:CLA:HMC3	14:A4:805:CLA:HED2	1.98	0.46
14:A5:804:CLA:HMC3	14:A5:806:CLA:HED2	1.97	0.46
1:A6:497:ALA:N	1:A6:498:PRO:CD	2.79	0.46
2:B1:427:TRP:CD1	14:B1:803:CLA:O1A	2.50	0.46
2:B2:658:PHE:CE2	2:B2:725:LEU:CD1	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B3:1804:CLA:H61	14:B3:1804:CLA:H41	1.67	0.46
2:B4:425:LEU:HD23	2:B4:425:LEU:HA	1.89	0.46
14:A4:841:CLA:H52	14:B4:842:CLA:H43	1.97	0.46
14:B5:1829:CLA:CGA	14:B5:1829:CLA:H3A	2.46	0.46
14:A5:842:CLA:H52	14:B5:1842:CLA:H43	1.98	0.46
2:B5:414:VAL:HG11	16:B5:1848:BCR:H401	1.96	0.46
2:B5:566:ASP:CG	3:C5:65:ARG:HH22	2.19	0.46
2:B5:625:TRP:HB3	14:B5:1803:CLA:H101	1.98	0.46
2:B6:350:LEU:HD13	14:B6:826:CLA:HAA1	1.97	0.46
3:C3:50:CYS:SG	18:C3:101:SF4:S4	3.14	0.46
10:L5:61:PRO:CB	14:L5:206:CLA:HBB1	2.42	0.46
12:X3:12:ARG:HE	17:X3:101:LHG:HC42	1.80	0.46
1:A1:100:TYR:HA	1:A1:144:PHE:CE1	2.51	0.46
1:A3:513:PHE:CE1	14:A3:827:CLA:HMC3	2.51	0.46
1:A4:647:ASN:HB2	2:B4:641:TYR:OH	2.16	0.46
14:A4:808:CLA:HBC2	14:A4:827:CLA:H141	1.95	0.46
1:A5:360:LEU:HD21	14:A5:830:CLA:CHC	2.46	0.46
14:A6:1651:CLA:CED	14:B6:804:CLA:H72	2.45	0.46
2:B1:535:THR:CG2	14:B1:802:CLA:HBD	2.35	0.46
2:B2:157:GLN:O	2:B2:161:ARG:HG3	2.16	0.46
2:B2:222:ALA:N	2:B2:223:PRO:CD	2.79	0.46
2:B2:400:ASP:OD1	4:D2:129:LYS:NZ	2.47	0.46
14:B2:832:CLA:C1	8:J2:29:PHE:CE2	2.99	0.46
2:B3:176:HIS:HB3	14:B3:1815:CLA:HHC	1.97	0.46
2:B3:535:THR:HG23	14:B3:1802:CLA:HBD	1.98	0.46
1:A4:706:TRP:CG	2:B4:419:GLU:HG3	2.51	0.46
2:B4:430:LEU:O	2:B4:434:PHE:CD1	2.68	0.46
2:B4:713:LEU:HD23	19:B4:851:LMG:H122	1.98	0.46
2:B4:436:THR:HG22	14:B4:803:CLA:H192	1.98	0.46
14:B4:804:CLA:H61	14:B4:804:CLA:H41	1.64	0.46
2:B4:189:TRP:CB	14:B4:816:CLA:HBB1	2.46	0.46
14:B5:1822:CLA:H3A	14:B5:1822:CLA:HBA2	1.70	0.46
2:B5:625:TRP:O	2:B5:629:TYR:HB3	2.16	0.46
14:A5:802:CLA:H41	2:B5:654:TRP:NE1	2.31	0.46
1:A6:702:GLU:CD	2:B6:551:LYS:HB2	2.35	0.46
14:B6:830:CLA:H3A	14:B6:830:CLA:HBA2	1.55	0.46
3:C1:65:ARG:HG2	3:C1:67:TYR:CZ	2.50	0.46
3:C2:28:VAL:HG12	4:D2:109:ARG:HB3	1.98	0.46
4:D2:71:GLN:NE2	4:D2:71:GLN:HA	2.31	0.46
4:D5:83:TYR:CE2	4:D5:93:LEU:HG	2.50	0.46
14:B5:1833:CLA:HBC3	16:F5:1302:BCR:H362	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J2:101:CLA:H3A	14:J2:101:CLA:HBA2	1.70	0.46
10:L1:57:PHE:CD1	10:L1:57:PHE:C	2.89	0.46
1:A2:473:ASP:OD1	10:L2:69:ARG:NH2	2.48	0.46
14:L3:203:CLA:HMB2	14:L3:203:CLA:H43	1.98	0.46
10:L6:35:PRO:HB2	10:L6:50:VAL:CG2	2.45	0.46
1:A1:178:PHE:CE2	14:A1:809:CLA:C2D	2.99	0.46
14:A3:817:CLA:H11	14:A3:817:CLA:ND	2.30	0.46
1:A4:200:HIS:ND1	14:A4:824:CLA:OBD	2.47	0.46
1:A4:377:MET:N	1:A4:378:PRO:CD	2.78	0.46
1:A5:90:MET:HE2	14:A5:828:CLA:CED	2.43	0.46
1:A6:396:HIS:O	1:A6:400:ILE:HG12	2.16	0.46
2:B1:275:HIS:CE1	14:B1:818:CLA:CHD	2.96	0.46
2:B2:279:ILE:HD11	14:B2:816:CLA:C3C	2.46	0.46
2:B2:547:ALA:O	2:B2:556:LYS:HD2	2.15	0.46
14:A2:1644:CLA:H52	14:B2:839:CLA:H43	1.97	0.46
16:B2:850:BCR:HC8	16:B2:850:BCR:H331	1.96	0.46
2:B3:340:HIS:CD2	14:B3:1807:CLA:OBD	2.68	0.46
2:B4:106:ALA:HB2	2:B4:114:ILE:CD1	2.46	0.46
2:B4:215:MET:HG2	14:B4:817:CLA:CGD	2.45	0.46
2:B5:688:HIS:NE2	14:B5:1842:CLA:CMD	2.79	0.46
3:C4:18:ARG:NH1	4:D4:103:GLU:HB3	2.31	0.46
16:F4:204:BCR:HC8	16:F4:204:BCR:H331	1.96	0.46
6:F6:101:ILE:HB	8:J6:14:LEU:CD1	2.46	0.46
8:J4:15:ALA:O	8:J4:19:MET:HB2	2.16	0.46
10:L2:131:SER:HB2	16:L2:201:BCR:H19C	1.97	0.46
16:L5:207:BCR:C8	16:L5:207:BCR:H331	2.46	0.46
16:L6:209:BCR:C8	16:L6:209:BCR:H331	2.46	0.46
2:B5:135:TYR:HB2	11:M5:3:LEU:HD11	1.98	0.46
1:A1:444:LEU:HD23	1:A1:551:LEU:HA	1.98	0.46
1:A1:583:ARG:HG3	3:C1:48:VAL:HB	1.98	0.46
1:A2:189:TRP:CH2	14:A2:1615:CLA:CHD	2.99	0.46
1:A2:204:LEU:HD11	14:A2:1631:CLA:H141	1.96	0.46
1:A2:654:LEU:HD11	14:A2:1602:CLA:H72	1.98	0.46
1:A4:433:VAL:HG21	14:A4:820:CLA:H192	1.96	0.46
1:A5:17:ASP:HB3	1:A5:20:PRO:HG3	1.98	0.46
14:A5:802:CLA:O2A	2:B5:657:LEU:HB3	2.16	0.46
14:A5:831:CLA:HBB1	14:A5:838:CLA:CBB	2.46	0.46
14:A6:1609:CLA:HBC2	14:A6:1628:CLA:H141	1.97	0.46
2:B1:303:MET:CE	14:B1:824:CLA:HED1	2.45	0.46
2:B2:500:LEU:O	2:B2:504:LEU:HG	2.15	0.46
2:B2:354:HIS:CE1	14:B2:825:CLA:NB	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:313:LYS:O	2:B3:314:VAL:CG2	2.56	0.46
2:B4:313:LYS:O	2:B4:314:VAL:HG13	2.16	0.46
2:B4:377:HIS:HE1	14:B4:829:CLA:C1D	2.29	0.46
14:A5:801:CLA:HMB3	14:B5:1804:CLA:OBD	2.15	0.46
2:B5:634:SER:O	2:B5:638:ILE:HB	2.15	0.46
2:B5:71:GLY:HA2	2:B5:86:ILE:HB	1.97	0.46
2:B6:589:MET:CE	2:B6:590:LEU:HD23	2.46	0.46
3:C5:15:GLN:HB3	3:C5:16:CYS:HA	1.98	0.46
10:L3:20:PRO:HB2	14:L3:202:CLA:HMD1	1.97	0.46
14:A3:834:CLA:H12	10:L3:62:TRP:NE1	2.31	0.46
10:L5:92:CYS:HB3	16:L5:207:BCR:C20	2.46	0.46
10:L6:142:PHE:CD1	14:L6:208:CLA:H12	2.46	0.46
1:A2:40:ARG:CD	13:P2:61:ASP:HA	2.43	0.46
1:A2:367:SER:OG	1:A2:397:HIS:O	2.33	0.46
1:A3:177:TRP:HB2	14:A3:811:CLA:CMC	2.43	0.46
1:A3:453:PHE:C	14:A3:834:CLA:HBB2	2.35	0.46
1:A5:33:HIS:CG	1:A5:34:PHE:N	2.84	0.46
14:A5:822:CLA:HBA2	14:A5:822:CLA:H3A	1.51	0.46
14:A6:1603:CLA:H71	14:A6:1640:CLA:CMC	2.45	0.46
1:A6:518:VAL:HG23	1:A6:525:ALA:HB3	1.98	0.46
1:A6:86:TRP:O	1:A6:90:MET:HG2	2.16	0.46
2:B1:274:HIS:HD1	14:B1:818:CLA:HMB1	1.80	0.46
2:B1:630:LEU:CD1	14:B1:804:CLA:H93	2.46	0.46
14:B1:808:CLA:H41	14:B1:808:CLA:H61	1.68	0.46
2:B1:290:TYR:HH	14:B1:820:CLA:CGD	2.27	0.46
2:B2:727:TYR:HB2	14:B2:801:CLA:CED	2.44	0.46
2:B2:582:PHE:CE2	14:B2:828:CLA:HMD2	2.51	0.46
14:A3:842:CLA:CMC	14:B3:1802:CLA:H71	2.45	0.46
2:B3:189:TRP:CB	14:B3:1816:CLA:HBB1	2.46	0.46
14:B3:1833:CLA:HBC3	16:F3:203:BCR:H362	1.96	0.46
14:B3:1837:CLA:HMB1	16:B3:1849:BCR:HC31	1.98	0.46
2:B3:220:GLY:O	2:B3:221:LEU:CB	2.63	0.46
2:B3:60:VAL:CG2	14:B3:1830:CLA:H11	2.45	0.46
2:B5:664:ALA:C	14:B5:1805:CLA:HBB1	2.37	0.46
14:B5:1808:CLA:H102	14:B5:1808:CLA:H151	1.96	0.46
14:B5:1819:CLA:HBA2	14:B5:1819:CLA:H3A	1.47	0.46
2:B5:718:HIS:HE1	14:B5:1843:CLA:CHA	2.29	0.46
14:B6:838:CLA:HMB2	14:B6:839:CLA:C2D	2.46	0.46
1:A1:42:PRO:HG3	6:F1:99:ILE:HD13	1.98	0.46
16:L4:206:BCR:H331	16:L4:206:BCR:C8	2.45	0.46
10:L4:79:LEU:HD22	10:L4:136:PHE:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M4:17:LEU:HB3	11:M4:18:PRO:HD3	1.97	0.46
1:A1:651:ARG:NH2	2:B1:643:PRO:HD3	2.31	0.46
1:A1:696:TYR:C	1:A1:696:TYR:CD2	2.89	0.46
14:A2:1623:CLA:HAA2	14:A2:1627:CLA:HBB1	1.98	0.46
1:A2:401:GLY:O	1:A2:405:VAL:HG23	2.15	0.46
1:A3:203:GLY:O	1:A3:207:LEU:HB2	2.16	0.46
1:A3:272:TRP:CD1	14:A3:817:CLA:HMB2	2.51	0.46
1:A4:231:VAL:O	1:A4:232:ALA:CB	2.57	0.46
1:A4:501:THR:C	1:A4:503:PRO:HD3	2.37	0.46
14:A6:1621:CLA:HMD1	14:A6:1622:CLA:HBB1	1.97	0.46
14:A6:1634:CLA:HMD2	14:A6:1635:CLA:HBB1	1.98	0.46
1:A6:244:LEU:C	1:A6:246:PRO:HD3	2.36	0.46
1:A6:453:PHE:C	14:A6:1633:CLA:HBB2	2.34	0.46
1:A6:483:GLN:HA	1:A6:484:PRO:HD3	1.84	0.46
2:B1:595:TRP:HZ2	14:B1:805:CLA:C1B	2.29	0.46
14:B3:1825:CLA:CBB	14:B3:1832:CLA:HMD2	2.46	0.46
2:B3:52:HIS:NE2	14:B3:1807:CLA:HMA1	2.30	0.46
14:A4:840:CLA:CMC	14:B4:802:CLA:H71	2.44	0.46
14:B4:837:CLA:HMB1	16:B4:849:BCR:HC31	1.98	0.46
2:B5:220:GLY:O	2:B5:221:LEU:HB2	2.15	0.46
2:B5:442:HIS:HB2	14:B5:1835:CLA:C1C	2.46	0.46
3:C3:17:VAL:HG22	3:C3:25:LEU:CB	2.45	0.46
14:I1:101:CLA:H18	16:I1:102:BCR:H362	1.98	0.46
14:B3:1842:CLA:H18	16:I3:101:BCR:H362	1.98	0.46
14:L1:205:CLA:HMB2	14:L1:205:CLA:H43	1.97	0.46
10:L5:28:LYS:O	10:L5:29:THR:C	2.55	0.46
10:L4:94:ALA:HB3	14:L6:206:CLA:HMD1	1.98	0.46
1:A1:677:LEU:HD11	2:B1:623:MET:HB2	1.98	0.45
14:A1:803:CLA:HMC3	14:A1:805:CLA:HED2	1.97	0.45
14:A2:1604:CLA:H71	14:A2:1643:CLA:CMC	2.45	0.45
14:A2:1611:CLA:HBC2	14:A2:1630:CLA:H141	1.97	0.45
1:A5:215:HIS:HB2	14:A5:814:CLA:CHC	2.46	0.45
14:A5:808:CLA:H3A	14:A5:808:CLA:HBA2	1.76	0.45
14:A5:821:CLA:CMD	14:A5:822:CLA:HBB1	2.46	0.45
1:A6:443:HIS:CD2	14:A6:1631:CLA:HMB1	2.52	0.45
2:B1:503:TRP:NE1	14:B1:835:CLA:CED	2.78	0.45
2:B1:288:HIS:C	14:B1:822:CLA:HAC2	2.37	0.45
14:B1:829:CLA:H12	16:B1:844:BCR:H393	1.98	0.45
14:B1:836:CLA:HBA2	14:B1:837:CLA:HMB3	1.97	0.45
14:B2:805:CLA:H143	14:B2:827:CLA:CBB	2.46	0.45
2:B3:64:LEU:HD11	16:B3:1847:BCR:H271	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:390:PHE:CD1	16:B3:1849:BCR:H373	2.50	0.45
2:B3:599:TYR:CD2	14:B3:1839:CLA:CMC	2.98	0.45
2:B4:281:VAL:HG22	16:B4:845:BCR:C35	2.46	0.45
2:B4:45:ILE:HG22	2:B4:49:HIS:NE2	2.31	0.45
2:B4:637:LEU:HD13	2:B4:733:ALA:HB3	1.98	0.45
2:B4:377:HIS:HB2	14:B4:829:CLA:CHB	2.46	0.45
14:B4:830:CLA:H12	16:B4:846:BCR:H393	1.98	0.45
2:B5:347:ILE:O	2:B5:351:VAL:HG23	2.17	0.45
2:B6:390:PHE:CZ	14:B6:825:CLA:HAB	2.51	0.45
14:B6:827:CLA:CGA	14:B6:827:CLA:H3A	2.46	0.45
14:B6:807:CLA:H91	19:B6:848:LMG:H401	1.97	0.45
3:C4:11:ILE:HD12	13:P4:39:SER:OG	2.16	0.45
6:F3:17:ARG:NE	6:F3:46:ASP:O	2.47	0.45
7:I6:15:ILE:HD11	14:I6:101:CLA:HAA1	1.98	0.45
10:L4:97:GLY:HA3	10:L4:117:TRP:HD1	1.81	0.45
11:M3:4:THR:N	11:M3:7:GLN:OE1	2.38	0.45
1:A1:244:LEU:C	1:A1:246:PRO:HD3	2.36	0.45
1:A1:36:ARG:HH22	13:P1:70:ILE:CB	2.03	0.45
1:A2:257:ASP:OD1	1:A2:258:TRP:N	2.49	0.45
1:A2:615:TRP:HB2	1:A2:653:PHE:CE1	2.51	0.45
1:A3:377:MET:N	1:A3:378:PRO:CD	2.80	0.45
1:A3:514:GLY:HA2	1:A3:528:PRO:HB3	1.97	0.45
1:A5:42:PRO:HG3	1:A5:47:TRP:CE3	2.51	0.45
1:A6:77:PHE:CE2	14:A6:1613:CLA:HED1	2.51	0.45
1:A6:455:SER:OG	1:A6:456:PHE:N	2.49	0.45
1:A6:553:LEU:HD21	1:A6:598:GLY:HA3	1.97	0.45
2:B1:275:HIS:HE1	14:B1:818:CLA:C4C	2.29	0.45
2:B1:533:LEU:O	2:B1:537:THR:OG1	2.27	0.45
2:B1:189:TRP:CE2	14:B1:819:CLA:C3D	2.99	0.45
14:B1:831:CLA:H3A	14:B1:831:CLA:HBA2	1.56	0.45
2:B3:166:TRP:CE2	14:B3:1813:CLA:HMA1	2.47	0.45
2:B3:174:LEU:HG	14:B3:1826:CLA:HMD3	1.96	0.45
2:B3:488:ALA:HA	14:B3:1837:CLA:C1D	2.46	0.45
16:B3:1846:BCR:H23C	16:B3:1846:BCR:C38	2.46	0.45
2:B4:625:TRP:O	2:B4:629:TYR:HB3	2.17	0.45
2:B4:433:GLY:HA3	14:B4:802:CLA:O1A	2.16	0.45
2:B4:622:LEU:CD1	14:B4:804:CLA:C1	2.70	0.45
14:B4:826:CLA:H61	14:B4:826:CLA:H41	1.76	0.45
16:B6:844:BCR:C38	16:B6:844:BCR:H23C	2.46	0.45
3:C4:11:ILE:HD13	13:P4:40:CYS:HA	1.98	0.45
14:B1:832:CLA:HBC3	16:F1:1302:BCR:H362	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F5:76:TRP:CH2	14:F5:1301:CLA:O1A	2.69	0.45
8:J2:27:ILE:HD13	16:J2:103:BCR:C11	2.45	0.45
6:F4:34:ARG:HD3	8:J4:35:ASP:CG	2.36	0.45
16:L3:206:BCR:H331	16:L3:206:BCR:C8	2.47	0.45
1:A1:313:HIS:CE1	16:A1:842:BCR:H363	2.50	0.45
14:A1:830:CLA:HBB1	14:A1:836:CLA:CBB	2.46	0.45
1:A3:718:GLN:HA	1:A3:719:PRO:HD3	1.89	0.45
14:A3:843:CLA:H52	14:B3:1842:CLA:H43	1.98	0.45
1:A4:257:ASP:OD1	1:A4:258:TRP:N	2.50	0.45
1:A4:292:LEU:HG	1:A4:378:PRO:O	2.16	0.45
1:A4:387:TYR:CE2	1:A4:622:TRP:CD1	3.04	0.45
16:A5:850:BCR:H362	14:B5:1804:CLA:C4	2.37	0.45
14:A6:1604:CLA:H2	14:A6:1611:CLA:H92	1.98	0.45
14:A6:1621:CLA:HAA2	14:A6:1625:CLA:HBB1	1.97	0.45
1:A6:19:ASP:N	1:A6:20:PRO:HD3	2.30	0.45
2:B1:189:TRP:CZ3	2:B1:192:HIS:CD2	3.04	0.45
2:B1:117:SER:HB3	14:B1:828:CLA:HAA2	1.98	0.45
14:B1:824:CLA:CBB	14:B1:831:CLA:HMD2	2.47	0.45
14:B2:807:CLA:HMB2	14:B2:807:CLA:H142	1.98	0.45
2:B2:361:TYR:OH	14:B2:827:CLA:OBD	2.20	0.45
2:B2:24:ILE:HG22	14:B2:828:CLA:H43	1.99	0.45
14:B3:1818:CLA:H41	14:B3:1818:CLA:H62	1.77	0.45
14:B3:1826:CLA:H61	14:B3:1828:CLA:H42	1.97	0.45
2:B3:184:VAL:HG23	14:B3:1822:CLA:HAC1	1.98	0.45
2:B4:222:ALA:HB3	2:B4:223:PRO:HD3	1.97	0.45
2:B5:598:PHE:HE1	14:B5:1803:CLA:HED2	1.82	0.45
2:B6:313:LYS:O	2:B6:314:VAL:CG2	2.58	0.45
2:B6:596:VAL:HG11	14:B6:837:CLA:HBB2	1.98	0.45
14:B5:1809:CLA:H102	16:I5:101:BCR:HC31	1.97	0.45
10:L1:38:ARG:NH2	14:L1:205:CLA:C4C	2.80	0.45
10:L6:58:LEU:HD22	10:L6:85:LEU:HD12	1.97	0.45
1:A2:709:ASN:CB	6:F2:136:ILE:HG23	2.45	0.45
1:A4:100:TYR:CE2	1:A4:104:LEU:HD11	2.51	0.45
1:A4:40:ARG:HG2	13:P4:60:SER:C	2.37	0.45
1:A4:466:ARG:HB2	1:A4:474:MET:SD	2.57	0.45
14:A4:803:CLA:H2	14:A4:810:CLA:H92	1.98	0.45
14:A5:802:CLA:O2D	2:B5:660:HIS:CD2	2.69	0.45
2:B1:288:HIS:O	14:B1:822:CLA:HAC2	2.16	0.45
14:A1:801:CLA:HMB3	14:B1:805:CLA:OBD	2.16	0.45
2:B1:59:TRP:CH2	14:B1:829:CLA:HMB2	2.52	0.45
14:B2:818:CLA:CMD	14:B2:820:CLA:HBB1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B2:843:BCR:C38	16:B2:843:BCR:H23C	2.47	0.45
2:B4:381:ILE:O	2:B4:385:LEU:HG	2.16	0.45
2:B4:430:LEU:HB3	14:B4:834:CLA:HED3	1.98	0.45
14:A4:801:CLA:HMB3	14:B4:804:CLA:OBD	2.16	0.45
14:B4:811:CLA:HMB3	14:B4:812:CLA:CHC	2.47	0.45
2:B4:214:THR:O	14:B4:817:CLA:HED1	2.17	0.45
14:B4:837:CLA:HBA2	14:B4:838:CLA:HMB3	1.98	0.45
2:B5:605:LEU:HD21	2:B5:633:ASN:ND2	2.32	0.45
2:B6:599:TYR:CE1	14:B6:837:CLA:CBC	2.99	0.45
1:A2:423:ALA:CA	4:D2:38:VAL:HG11	2.43	0.45
4:D3:58:PHE:HB3	4:D3:63:GLN:OE1	2.16	0.45
6:F5:37:ARG:O	6:F5:40:GLN:HG2	2.17	0.45
14:J3:101:CLA:HBA2	14:J3:101:CLA:H3A	1.69	0.45
8:J3:21:ILE:HA	14:J3:101:CLA:HBB2	1.98	0.45
1:A1:143:LEU:HD22	1:A1:147:TRP:CH2	2.51	0.45
1:A1:649:TRP:O	1:A1:653:PHE:HB3	2.17	0.45
1:A1:686:SER:HB3	1:A1:734:HIS:CB	2.47	0.45
1:A2:348:LEU:CD1	14:A2:1627:CLA:HMC2	2.47	0.45
1:A2:475:PHE:HA	1:A2:480:ILE:O	2.17	0.45
1:A3:86:TRP:O	1:A3:90:MET:HG2	2.16	0.45
1:A4:360:LEU:HD21	14:A4:829:CLA:CHC	2.47	0.45
1:A5:544:PHE:O	1:A5:548:VAL:HG23	2.16	0.45
16:A6:1647:BCR:H382	16:A6:1647:BCR:H23C	1.99	0.45
2:B1:137:GLY:HA2	16:B1:845:BCR:H381	1.99	0.45
2:B1:343:CYS:SG	14:B1:827:CLA:H92	2.57	0.45
14:A2:1602:CLA:HMB3	14:B2:802:CLA:OBD	2.16	0.45
14:B2:822:CLA:CBB	14:B2:829:CLA:HMD2	2.47	0.45
14:B3:1809:CLA:H102	16:I3:101:BCR:HC31	1.98	0.45
2:B4:276:HIS:CD2	14:B4:820:CLA:NC	2.83	0.45
2:B4:605:LEU:HD12	2:B4:605:LEU:HA	1.88	0.45
14:B4:825:CLA:CBB	14:B4:832:CLA:HMD2	2.47	0.45
14:B5:1830:CLA:H12	16:B5:1846:BCR:H393	1.99	0.45
2:B6:189:TRP:CZ3	2:B6:192:HIS:CD2	3.05	0.45
17:B6:849:LHG:HC2	12:X6:12:ARG:HH21	1.82	0.45
5:E4:68:VAL:O	5:E4:69:ALA:O	2.34	0.45
14:B6:840:CLA:H18	16:I6:102:BCR:H362	1.99	0.45
10:L1:125:PHE:C	10:L1:125:PHE:CD2	2.89	0.45
14:B6:840:CLA:H43	14:L6:203:CLA:H52	1.98	0.45
1:A1:281:PHE:CE1	14:A1:817:CLA:HAB	2.51	0.45
1:A1:36:ARG:HH12	13:P1:70:ILE:HB	1.81	0.45
14:A2:1624:CLA:HBA2	14:A2:1624:CLA:H3A	1.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:691:PHE:HB2	14:A2:1604:CLA:CBC	2.47	0.45
1:A3:341:HIS:HE1	17:A3:854:LHG:HC11	1.81	0.45
1:A3:302:LEU:HD11	14:A3:817:CLA:CBB	2.46	0.45
1:A4:366:LEU:HD11	14:A4:818:CLA:H71	1.97	0.45
14:A4:820:CLA:HAA2	14:A4:824:CLA:HBB1	1.99	0.45
1:A4:602:MET:HG2	14:A4:825:CLA:HBC1	1.99	0.45
1:A5:484:PRO:HB3	14:A5:837:CLA:HED3	1.98	0.45
2:B1:186:SER:HB2	14:B1:819:CLA:CMC	2.46	0.45
2:B1:427:TRP:CZ2	14:B1:832:CLA:CBB	3.00	0.45
2:B1:600:TRP:HB2	14:B1:838:CLA:HMC1	1.98	0.45
2:B1:379:GLN:OE1	14:B1:826:CLA:CMD	2.65	0.45
2:B2:313:LYS:O	2:B2:314:VAL:CG2	2.57	0.45
2:B2:525:VAL:HG12	14:B2:801:CLA:H141	1.99	0.45
2:B3:438:GLY:HA3	14:B3:1835:CLA:CBB	2.47	0.45
2:B4:651:VAL:HG13	14:B4:811:CLA:HAC1	1.98	0.45
14:B5:1818:CLA:H41	14:B5:1818:CLA:H62	1.78	0.45
2:B5:599:TYR:CZ	14:B5:1839:CLA:CBC	2.99	0.45
7:I1:31:PHE:O	7:I1:35:GLU:HG2	2.16	0.45
14:J4:101:CLA:HBA2	14:J4:101:CLA:H3A	1.69	0.45
8:J5:40:PRO:O	8:J5:41:LEU:HB2	2.17	0.45
10:L1:90:THR:HG21	10:L1:125:PHE:HB2	1.98	0.45
10:L5:64:LYS:HB2	14:L5:206:CLA:HMB3	1.99	0.45
10:L6:142:PHE:HD1	14:L6:208:CLA:H43	1.82	0.45
10:L6:92:CYS:HB3	16:L6:209:BCR:C19	2.47	0.45
1:A1:79:HIS:NE2	14:A1:804:CLA:HMA1	2.32	0.45
1:A1:45:THR:HG21	14:A1:837:CLA:C4B	2.47	0.45
14:A2:1602:CLA:CGD	14:A2:1602:CLA:HAA2	2.46	0.45
1:A2:379:PRO:HD2	1:A2:383:LEU:CD2	2.47	0.45
1:A3:399:TRP:CZ3	1:A3:740:ILE:HG12	2.52	0.45
1:A4:212:TRP:HA	14:A4:813:CLA:HBB1	1.99	0.45
14:A4:808:CLA:CBB	14:B4:835:CLA:HMD2	2.47	0.45
14:A4:840:CLA:O1A	14:A4:840:CLA:H2	2.17	0.45
1:A5:16:VAL:HG12	1:A5:17:ASP:N	2.32	0.45
1:A5:592:TRP:NE1	14:A5:830:CLA:HMD1	2.32	0.45
14:A5:806:CLA:H62	14:A5:806:CLA:H41	1.80	0.45
1:A5:303:ALA:HB2	14:A5:818:CLA:CBB	2.44	0.45
1:A6:390:GLN:HA	1:A6:390:GLN:HE21	1.81	0.45
2:B1:222:ALA:HB3	2:B1:223:PRO:HD3	1.97	0.45
2:B1:41:LEU:O	2:B1:45:ILE:HG12	2.17	0.45
2:B1:229:TRP:HB2	14:B1:817:CLA:HBA2	1.99	0.45
14:B1:817:CLA:H3A	14:B1:817:CLA:HBA2	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B1:853:CLA:HBC2	1:A2:332:HIS:HA	1.99	0.45
2:B1:90:ILE:HB	2:B1:111:PRO:HB2	1.99	0.45
2:B2:497:ASN:HB3	2:B2:500:LEU:HB2	1.99	0.45
1:A2:650:LEU:HD22	2:B2:657:LEU:HD21	1.98	0.45
14:B2:816:CLA:HBA2	14:B2:816:CLA:H3A	1.44	0.45
14:B3:1843:CLA:H161	7:I3:27:MET:HE3	1.99	0.45
14:B3:1822:CLA:HBB1	16:B3:1845:BCR:H14C	1.98	0.45
2:B3:195:HIS:O	2:B3:206:VAL:HG11	2.16	0.45
2:B4:128:MET:HE3	2:B4:134:LEU:HD23	1.99	0.45
2:B4:337:LEU:HD21	14:B4:831:CLA:C1B	2.47	0.45
2:B4:642:ASN:HB2	2:B4:643:PRO:CD	2.46	0.45
2:B5:529:ILE:HG21	14:B5:1839:CLA:HAB	1.99	0.45
2:B5:60:VAL:HG22	14:B5:1830:CLA:H11	1.99	0.45
2:B6:376:THR:HG23	2:B6:597:THR:HG21	1.99	0.45
2:B6:155:HIS:CE1	14:B6:811:CLA:C1A	2.99	0.45
14:B6:828:CLA:H12	16:B6:844:BCR:H393	1.99	0.45
4:D2:31:TRP:NE1	4:D2:49:MET:SD	2.87	0.45
14:I6:101:CLA:H102	16:I6:102:BCR:HC31	1.99	0.45
14:B2:809:CLA:H91	14:L3:205:CLA:H93	1.99	0.45
10:L4:54:HIS:O	10:L4:58:LEU:HG	2.17	0.45
14:B3:1801:CLA:HMA2	14:M3:1601:CLA:HBD	1.99	0.45
1:A1:366:LEU:HD11	14:A1:818:CLA:H71	1.99	0.45
1:A1:612:HIS:CE1	14:A1:834:CLA:C2C	3.00	0.45
1:A3:293:TRP:HB2	1:A3:296:ASP:CG	2.37	0.45
1:A3:387:TYR:N	1:A3:388:PRO:CD	2.80	0.45
1:A3:691:PHE:N	1:A3:691:PHE:HD1	2.14	0.45
14:A3:820:CLA:HBA2	14:A3:820:CLA:H3A	1.87	0.45
1:A3:352:TRP:NE1	14:A3:825:CLA:H201	2.32	0.45
1:A4:75:ALA:HB1	14:A4:804:CLA:HBB1	1.99	0.45
14:A5:810:CLA:H3A	14:A5:810:CLA:HBA2	1.70	0.45
14:A5:826:CLA:HAB	16:A5:849:BCR:H311	1.98	0.45
1:A6:352:TRP:HB3	14:A6:1605:CLA:HAC1	1.98	0.45
1:A6:501:THR:C	1:A6:503:PRO:HD3	2.37	0.45
1:A6:691:PHE:HB2	14:A6:1603:CLA:CBC	2.46	0.45
2:B1:164:LEU:HD11	2:B1:168:LYS:HE2	1.99	0.45
2:B1:625:TRP:CH2	14:B1:804:CLA:H142	2.52	0.45
2:B1:339:TRP:HZ3	14:B1:824:CLA:HBC2	1.80	0.45
14:B1:828:CLA:H3A	14:B1:828:CLA:CGA	2.47	0.45
14:B1:836:CLA:HMB1	16:B1:847:BCR:HC31	1.98	0.45
2:B2:521:GLY:O	2:B2:525:VAL:HG22	2.17	0.45
14:B3:1808:CLA:H91	19:B3:1850:LMG:H401	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:350:LEU:HD23	14:B4:820:CLA:H41	1.98	0.45
14:B4:810:CLA:O1A	14:B4:829:CLA:HBD	2.16	0.45
2:B4:174:LEU:CD2	14:B4:826:CLA:C2D	2.94	0.45
2:B6:156:LEU:HA	2:B6:156:LEU:HD23	1.87	0.45
2:B6:499:TRP:CH2	14:B6:835:CLA:HED3	2.52	0.45
14:B6:816:CLA:H41	14:B6:816:CLA:H62	1.78	0.45
2:B6:350:LEU:N	14:B6:825:CLA:HED3	2.32	0.45
3:C1:25:LEU:HA	3:C1:40:SER:O	2.17	0.45
3:C5:14:THR:C	3:C5:15:GLN:O	2.55	0.45
1:A4:564:ARG:NH2	4:D4:16:GLY:O	2.48	0.45
14:B1:809:CLA:H102	16:I1:102:BCR:HC31	1.98	0.45
10:L3:115:GLU:O	10:L3:118:SER:OG	2.30	0.45
14:L4:203:CLA:HBA1	10:L5:87:LEU:HD21	1.97	0.45
10:L5:68:LEU:HD13	10:L5:73:VAL:HG23	1.98	0.45
1:A1:590:SER:OG	1:A1:593:ASP:OD2	2.29	0.45
16:A2:1651:BCR:H382	16:A2:1651:BCR:H23C	1.99	0.45
14:A2:1628:CLA:HAB	16:A2:1651:BCR:H311	1.98	0.45
1:A2:219:VAL:C	1:A2:222:PRO:HD2	2.37	0.45
1:A3:74:SER:OG	1:A3:180:TYR:HB2	2.17	0.45
1:A5:497:ALA:N	1:A5:498:PRO:CD	2.80	0.45
1:A5:642:SER:O	1:A5:648:GLY:HA3	2.17	0.45
1:A6:642:SER:O	1:A6:648:GLY:HA3	2.16	0.45
2:B1:313:LYS:O	2:B1:314:VAL:CG2	2.57	0.45
2:B2:361:TYR:O	2:B2:364:ILE:HG22	2.16	0.45
2:B2:580:ASP:OD1	2:B2:712:ARG:NH1	2.50	0.45
2:B2:318:PHE:CG	14:B2:821:CLA:HAB	2.52	0.45
2:B3:181:LEU:HG	14:B3:1815:CLA:H43	1.99	0.45
14:B3:1819:CLA:HBA2	14:B3:1819:CLA:H3A	1.47	0.45
14:B3:1821:CLA:CMD	14:B3:1823:CLA:HBB1	2.47	0.45
2:B3:533:LEU:HD22	14:B3:1827:CLA:C4C	2.47	0.45
2:B4:176:HIS:HB3	14:B4:815:CLA:HHC	1.99	0.45
14:B4:821:CLA:CMD	14:B4:823:CLA:HBB1	2.45	0.45
2:B4:184:VAL:CG1	16:B4:846:BCR:H352	2.47	0.45
2:B5:678:GLN:HA	2:B5:681:ILE:HD12	1.99	0.45
2:B5:685:VAL:HG11	3:C5:80:TYR:CD1	2.51	0.45
2:B6:480:LEU:C	2:B6:482:SER:N	2.69	0.45
2:B6:177:HIS:ND1	14:B6:824:CLA:O1D	2.29	0.45
3:C2:25:LEU:HA	3:C2:40:SER:O	2.17	0.45
3:C6:25:LEU:HA	3:C6:40:SER:O	2.17	0.45
3:C1:28:VAL:HG12	4:D1:109:ARG:CB	2.47	0.45
6:F3:37:ARG:HD2	8:J3:40:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L6:203:CLA:HHC	14:L6:203:CLA:HBB1	1.98	0.45
14:A1:801:CLA:CGD	14:A1:801:CLA:HAA2	2.47	0.45
14:A1:818:CLA:O1A	14:A1:828:CLA:HMD1	2.17	0.45
14:A1:833:CLA:H3A	14:A1:833:CLA:HBA2	1.79	0.45
14:A2:1622:CLA:HBA2	14:A2:1622:CLA:H3A	1.87	0.45
1:A2:86:TRP:O	1:A2:90:MET:HG2	2.16	0.45
1:A3:642:SER:O	1:A3:648:GLY:HA3	2.17	0.45
1:A3:444:LEU:HD13	14:A3:839:CLA:C4B	2.47	0.45
1:A4:100:TYR:HA	1:A4:144:PHE:CE1	2.51	0.45
1:A4:642:SER:O	1:A4:648:GLY:HA3	2.17	0.45
1:A5:177:TRP:HB2	14:A5:811:CLA:CMC	2.45	0.45
1:A5:600:PHE:CZ	1:A5:732:VAL:HG23	2.52	0.45
2:B1:275:HIS:O	2:B1:279:ILE:HG12	2.17	0.45
14:B1:817:CLA:H41	14:B1:817:CLA:H62	1.76	0.45
2:B2:235:ASN:N	2:B2:235:ASN:OD1	2.48	0.45
2:B2:339:TRP:HZ3	14:B2:822:CLA:HBC2	1.82	0.45
14:B2:807:CLA:O1A	14:B2:826:CLA:HBD	2.17	0.45
14:A2:1611:CLA:CBB	14:B2:832:CLA:HMD2	2.47	0.45
14:B3:1806:CLA:HMB2	16:M3:1602:BCR:HC42	1.98	0.45
2:B3:21:TRP:CE2	14:B3:1842:CLA:HMB1	2.45	0.45
2:B3:361:TYR:O	2:B3:364:ILE:HG22	2.17	0.45
2:B3:416:GLN:O	6:F3:141:ARG:NH2	2.50	0.45
2:B3:652:TRP:CH2	14:B3:1810:CLA:HBC2	2.52	0.45
2:B4:281:VAL:HG22	16:B4:845:BCR:H352	1.98	0.45
2:B4:171:GLU:HB3	2:B4:290:TYR:HB3	1.99	0.45
2:B4:669:PHE:HA	15:B4:844:PQN:O1	2.16	0.45
2:B5:434:PHE:CE2	14:B5:1802:CLA:H2	2.52	0.45
2:B5:60:VAL:HG21	14:B5:1830:CLA:H42	1.99	0.45
2:B5:220:GLY:O	2:B5:221:LEU:CB	2.64	0.45
14:B6:807:CLA:H143	14:B6:828:CLA:CBB	2.47	0.45
1:A4:583:ARG:HA	3:C4:76:MET:CA	2.47	0.45
5:E1:44:ASN:OD1	5:E1:55:VAL:HB	2.17	0.45
6:F2:77:ILE:HG12	14:F2:202:CLA:ND	2.31	0.45
8:J4:27:ILE:HG21	16:J4:104:BCR:C34	2.47	0.45
2:B5:458:ILE:HD11	16:J5:105:BCR:H341	1.98	0.45
10:L4:124:PHE:CE1	16:L4:206:BCR:H292	2.51	0.45
10:L4:6:LYS:HB2	10:L4:7:PRO:HD2	1.99	0.45
1:A1:475:PHE:HA	1:A1:480:ILE:O	2.16	0.44
1:A1:542:HIS:HB3	14:A1:834:CLA:HBB1	1.99	0.44
1:A2:303:ALA:HB2	14:A2:1620:CLA:CBB	2.47	0.44
1:A2:377:MET:N	1:A2:378:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:221:LEU:HD11	1:A3:295:SER:HA	1.99	0.44
1:A3:675:LEU:HD23	1:A3:744:TRP:HZ3	1.82	0.44
14:A3:821:CLA:HAA2	14:A3:825:CLA:HBB1	1.98	0.44
14:A3:835:CLA:HMD2	14:A3:836:CLA:HBB1	1.99	0.44
1:A4:511:VAL:HB	1:A4:526:MET:HG3	1.99	0.44
1:A5:577:PRO:C	1:A5:578:CYS:SG	2.95	0.44
1:A5:651:ARG:HB2	2:B5:638:ILE:CG2	2.44	0.44
14:A5:801:CLA:HAA2	14:A5:801:CLA:CGD	2.47	0.44
2:B1:427:TRP:CE2	14:B1:832:CLA:CBB	3.00	0.44
2:B2:216:PRO:HD2	14:B2:814:CLA:C3D	2.48	0.44
2:B2:663:TRP:CE2	14:B2:801:CLA:HBA2	2.52	0.44
2:B2:537:THR:HG21	14:B2:824:CLA:HBB2	1.99	0.44
2:B3:345:GLY:HA2	2:B3:385:LEU:HD12	2.00	0.44
2:B4:554:PRO:HD2	3:C4:61:PHE:CE1	2.53	0.44
14:B5:1801:CLA:HBA1	14:B5:1801:CLA:H3A	1.79	0.44
2:B5:603:LYS:HD3	14:B5:1839:CLA:HBC1	1.99	0.44
2:B5:430:LEU:HG	2:B5:434:PHE:CE1	2.52	0.44
2:B6:313:LYS:O	2:B6:314:VAL:HG13	2.18	0.44
3:C3:45:GLU:OE1	3:C3:45:GLU:N	2.40	0.44
1:A1:718:GLN:NE2	5:E1:15:TYR:OH	2.50	0.44
6:F4:77:ILE:HG23	14:F4:202:CLA:C1D	2.47	0.44
16:I1:103:BCR:C8	16:I1:103:BCR:H331	2.48	0.44
8:J6:27:ILE:HG22	16:J6:1105:BCR:H343	1.99	0.44
10:L5:54:HIS:HE1	14:L5:205:CLA:C4D	2.30	0.44
1:A4:40:ARG:NH1	13:P4:63:SER:HB3	2.31	0.44
1:A2:387:TYR:N	1:A2:388:PRO:CD	2.80	0.44
1:A2:565:LEU:HD11	1:A2:583:ARG:HB3	2.00	0.44
14:A3:821:CLA:HMD1	14:A3:822:CLA:HBB1	1.97	0.44
1:A4:244:LEU:C	1:A4:246:PRO:HD3	2.37	0.44
14:A4:805:CLA:H62	14:A4:805:CLA:H41	1.79	0.44
14:A6:1602:CLA:CGD	14:A6:1602:CLA:HAA2	2.47	0.44
14:A6:1606:CLA:H41	14:A6:1606:CLA:H62	1.80	0.44
1:A6:221:LEU:HD11	1:A6:295:SER:HB3	1.99	0.44
14:B1:854:CLA:C3B	7:I1:20:TRP:HE1	2.30	0.44
2:B2:504:LEU:HA	2:B2:507:ILE:HG22	2.00	0.44
2:B2:298:HIS:ND1	14:B2:821:CLA:OBD	2.50	0.44
2:B3:377:HIS:HE2	14:B3:1830:CLA:C1B	2.30	0.44
2:B3:60:VAL:HG21	14:B3:1830:CLA:H42	1.98	0.44
2:B3:75:GLN:N	2:B3:75:GLN:OE1	2.50	0.44
1:A4:651:ARG:NH2	2:B4:643:PRO:HD3	2.32	0.44
2:B5:630:LEU:HD13	14:B5:1803:CLA:C2D	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B5:1840:CLA:HMB2	14:B5:1841:CLA:C2D	2.46	0.44
2:B5:256:PHE:CD2	14:B5:1819:CLA:HMB2	2.53	0.44
2:B5:582:PHE:CE2	14:B5:1831:CLA:HMD2	2.52	0.44
2:B6:117:SER:O	14:B6:828:CLA:HED3	2.17	0.44
2:B6:525:VAL:HG12	14:B6:804:CLA:H141	1.99	0.44
3:C3:17:VAL:HG22	3:C3:25:LEU:HB2	1.98	0.44
3:C5:25:LEU:HD23	3:C5:41:SER:HB3	1.98	0.44
5:E2:68:VAL:O	5:E2:69:ALA:O	2.35	0.44
6:F2:110:MET:HB3	14:F2:202:CLA:HED2	1.99	0.44
8:J2:26:LEU:HD23	16:J2:102:BCR:HC7	1.99	0.44
10:L1:98:LEU:CD2	10:L2:41:LEU:HD21	2.44	0.44
10:L5:48:LEU:HD13	14:L5:204:CLA:HED2	2.00	0.44
5:E3:37:ILE:CD1	13:P3:41:ARG:HD2	2.45	0.44
2:B1:465:PHE:CE1	12:X1:30:TYR:HA	2.52	0.44
1:A1:177:TRP:HB2	14:A1:810:CLA:CMC	2.45	0.44
1:A1:603:TYR:OH	1:A1:739:GLY:HA3	2.17	0.44
1:A4:484:PRO:HB3	14:A4:836:CLA:HED3	1.99	0.44
1:A4:547:HIS:CE1	14:A4:837:CLA:C1A	3.00	0.44
16:A4:848:BCR:H23C	16:A4:848:BCR:H382	1.99	0.44
14:A4:853:CLA:H3A	14:A4:853:CLA:HBA2	1.75	0.44
14:A5:819:CLA:O1A	14:A5:829:CLA:HMD1	2.17	0.44
1:A6:675:LEU:HD11	14:A6:1628:CLA:H143	1.99	0.44
2:B1:105:GLN:O	2:B1:106:ALA:C	2.56	0.44
2:B1:713:LEU:HD11	19:B1:850:LMG:H342	1.99	0.44
2:B1:52:HIS:ND1	14:B1:807:CLA:H3A	2.33	0.44
2:B1:52:HIS:ND1	14:B1:807:CLA:HMA1	2.27	0.44
14:B1:811:CLA:H102	14:B1:828:CLA:H193	1.99	0.44
14:B1:839:CLA:HMB2	14:B1:840:CLA:C2D	2.46	0.44
2:B2:313:LYS:O	2:B2:314:VAL:HG13	2.17	0.44
2:B2:599:TYR:CZ	14:B2:836:CLA:HBC2	2.52	0.44
2:B2:7:PHE:CZ	2:B2:27:ALA:HA	2.53	0.44
14:B2:819:CLA:HBA2	14:B2:819:CLA:H3A	1.70	0.44
2:B3:125:THR:CG2	14:B3:1820:CLA:HED1	2.47	0.44
2:B3:182:PHE:N	2:B3:182:PHE:CD2	2.85	0.44
2:B3:711:ALA:CB	15:B3:1844:PQN:C8	2.95	0.44
2:B3:376:THR:HG23	2:B3:597:THR:HG21	1.98	0.44
14:B4:808:CLA:H143	14:B4:830:CLA:CBB	2.47	0.44
2:B4:288:HIS:O	14:B4:822:CLA:HED1	2.18	0.44
14:B4:829:CLA:H3A	14:B4:829:CLA:CGA	2.46	0.44
14:B4:840:CLA:HMB2	14:B4:841:CLA:C2D	2.48	0.44
2:B5:166:TRP:CZ2	14:B5:1815:CLA:CAC	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B5:433:GLY:HA3	14:B5:1802:CLA:CGA	2.47	0.44
2:B6:601:HIS:HB3	2:B6:629:TYR:OH	2.17	0.44
4:D1:32:THR:HA	4:D1:52:GLY:O	2.17	0.44
1:A5:714:ALA:O	6:F5:89:ARG:NH2	2.49	0.44
10:L2:125:PHE:O	10:L2:129:MET:HG2	2.18	0.44
10:L3:35:PRO:HG3	14:L3:204:CLA:HED2	2.00	0.44
1:A5:453:PHE:C	14:L5:203:CLA:HBB2	2.36	0.44
14:L5:204:CLA:H43	14:L5:204:CLA:HMB2	1.99	0.44
10:L5:43:PRO:HB2	10:L5:119:GLN:HB2	2.00	0.44
1:A1:642:SER:O	1:A1:648:GLY:HA3	2.17	0.44
1:A2:28:TRP:CZ2	14:A2:1606:CLA:H11	2.53	0.44
1:A2:642:SER:O	1:A2:648:GLY:HA3	2.17	0.44
1:A2:683:TRP:O	1:A2:686:SER:OG	2.34	0.44
1:A4:682:ILE:HD11	16:A4:849:BCR:C15	2.47	0.44
1:A4:683:TRP:CG	14:A4:801:CLA:HMA2	2.53	0.44
1:A5:300:HIS:O	1:A5:304:ILE:HG12	2.16	0.44
1:A5:410:ALA:HA	1:A5:595:VAL:HG21	1.99	0.44
1:A6:98:SER:HB2	1:A6:113:SER:O	2.17	0.44
1:A6:336:PHE:CB	17:A6:1650:LHG:HC41	2.44	0.44
1:A6:387:TYR:CE1	1:A6:622:TRP:HB3	2.52	0.44
1:A6:544:PHE:CE2	14:B6:802:CLA:HBB1	2.52	0.44
2:B1:463:ALA:HB2	14:B1:839:CLA:O2D	2.17	0.44
1:A1:650:LEU:HD23	2:B1:638:ILE:HD11	1.98	0.44
2:B1:137:GLY:CA	16:B1:845:BCR:H381	2.47	0.44
2:B2:176:HIS:CE1	14:B2:819:CLA:HMD1	2.52	0.44
2:B3:182:PHE:N	2:B3:182:PHE:HD2	2.15	0.44
2:B4:531:LEU:CD1	14:B4:802:CLA:O1A	2.65	0.44
14:B4:842:CLA:H18	16:I4:101:BCR:H362	1.99	0.44
2:B5:121:HIS:CD2	2:B5:364:ILE:HA	2.52	0.44
14:B5:1837:CLA:HMB1	16:B5:1849:BCR:HC31	1.99	0.44
2:B5:430:LEU:HD13	14:B5:1802:CLA:HED3	1.99	0.44
5:E6:57:THR:HG21	13:P6:42:ALA:HA	1.98	0.44
6:F5:65:ILE:CD1	14:J5:102:CLA:HMB3	2.47	0.44
14:A1:839:CLA:H62	14:A1:839:CLA:H41	1.68	0.44
1:A2:352:TRP:CD1	14:A2:1627:CLA:H201	2.53	0.44
1:A3:352:TRP:CE2	14:A3:825:CLA:C18	2.96	0.44
14:A3:834:CLA:H11	10:L3:62:TRP:CZ2	2.52	0.44
1:A3:447:VAL:HG21	14:A3:839:CLA:C2C	2.47	0.44
14:A4:834:CLA:H3A	14:A4:834:CLA:HBA2	1.79	0.44
1:A5:543:ALA:HB1	14:A5:837:CLA:HMB3	2.00	0.44
1:A6:177:TRP:HB2	14:A6:1611:CLA:CMC	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:503:TRP:HE1	14:B1:835:CLA:HED1	1.82	0.44
16:B1:852:BCR:H21C	8:J1:36:LEU:HD22	1.98	0.44
2:B2:171:GLU:HB3	2:B2:290:TYR:HB3	2.00	0.44
14:B2:806:CLA:C4	7:I2:14:PHE:CE1	2.98	0.44
2:B2:166:TRP:CE2	14:B2:812:CLA:HAC2	2.53	0.44
2:B3:157:GLN:O	2:B3:161:ARG:HG3	2.17	0.44
2:B4:456:ILE:HG22	2:B4:458:ILE:CD1	2.48	0.44
2:B4:582:PHE:CZ	14:B4:831:CLA:HMD2	2.53	0.44
14:B4:843:CLA:H161	7:I4:27:MET:HE3	1.98	0.44
14:B5:1808:CLA:H41	14:B5:1808:CLA:H61	1.70	0.44
16:B5:1846:BCR:C38	16:B5:1846:BCR:H23C	2.48	0.44
2:B5:480:LEU:C	2:B5:482:SER:N	2.71	0.44
2:B6:360:PRO:HG3	14:B6:818:CLA:CBA	2.48	0.44
14:B6:808:CLA:O1A	14:B6:827:CLA:HBD	2.17	0.44
14:B6:824:CLA:H61	14:B6:824:CLA:H41	1.76	0.44
1:A2:582:GLY:CA	3:C2:48:VAL:O	2.65	0.44
3:C4:25:LEU:HA	3:C4:40:SER:O	2.18	0.44
14:A4:802:CLA:HED1	8:J4:12:PRO:HA	1.99	0.44
6:F6:61:GLY:H	8:J6:41:LEU:HD11	1.81	0.44
10:L1:7:PRO:HB3	10:L1:12:PRO:HA	1.98	0.44
1:A2:453:PHE:C	14:L2:202:CLA:HBB2	2.37	0.44
10:L2:30:PHE:O	10:L2:34:LEU:HD13	2.17	0.44
11:M6:17:LEU:HB3	11:M6:18:PRO:HD3	1.99	0.44
14:A1:828:CLA:HBB1	14:A1:828:CLA:HMB1	1.98	0.44
1:A2:201:LEU:HD21	14:A2:1623:CLA:C4B	2.47	0.44
1:A2:352:TRP:CE2	14:A2:1627:CLA:H18	2.52	0.44
1:A3:501:THR:C	1:A3:503:PRO:HD3	2.38	0.44
14:A3:843:CLA:HHC	14:A3:843:CLA:HBB1	1.99	0.44
1:A3:99:ASN:HB3	1:A3:134:PHE:CG	2.53	0.44
1:A4:303:ALA:HB2	14:A4:817:CLA:CBB	2.47	0.44
14:A4:830:CLA:HMB2	14:A4:831:CLA:C2D	2.48	0.44
1:A5:19:ASP:N	1:A5:20:PRO:HD3	2.33	0.44
14:A5:831:CLA:HMB2	14:A5:832:CLA:C2D	2.47	0.44
1:A6:439:ALA:HA	2:B6:686:TRP:CH2	2.52	0.44
14:B1:821:CLA:HBA2	14:B1:821:CLA:H3A	1.70	0.44
2:B2:526:HIS:ND1	14:B2:837:CLA:HED3	2.33	0.44
2:B3:582:PHE:CE2	14:B3:1831:CLA:HMD2	2.53	0.44
2:B4:174:LEU:HD21	14:B4:826:CLA:C3D	2.47	0.44
2:B4:25:ALA:CB	19:B4:851:LMG:H121	2.38	0.44
2:B4:90:ILE:HB	2:B4:111:PRO:HB2	1.98	0.44
2:B5:375:TYR:CE2	2:B5:600:TRP:CD1	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B5:716:LEU:O	2:B5:720:SER:OG	2.25	0.44
2:B5:637:LEU:HD22	2:B5:730:PHE:HA	1.99	0.44
2:B6:222:ALA:N	2:B6:223:PRO:CD	2.80	0.44
2:B6:393:GLY:HA2	16:B6:847:BCR:H393	1.99	0.44
1:A6:706:TRP:CG	2:B6:419:GLU:HG3	2.52	0.44
2:B6:425:LEU:HA	2:B6:425:LEU:HD23	1.86	0.44
2:B6:298:HIS:ND1	14:B6:822:CLA:OBD	2.50	0.44
14:B6:824:CLA:H61	14:B6:826:CLA:H42	1.98	0.44
3:C5:14:THR:HB	3:C5:15:GLN:O	2.17	0.44
1:A6:567:PRO:HB3	4:D6:42:PRO:HB2	2.00	0.44
5:E4:59:ASN:N	5:E4:59:ASN:OD1	2.49	0.44
6:F1:103:VAL:HG12	6:F1:107:ILE:HD11	2.00	0.44
14:B2:839:CLA:H18	16:I2:101:BCR:H362	1.99	0.44
7:I6:12:TRP:CE2	10:L5:149:MET:HG3	2.52	0.44
14:A1:830:CLA:HMB2	14:L1:201:CLA:C2D	2.47	0.44
5:E2:3:ARG:HH12	13:P2:31:GLU:HA	1.83	0.44
1:A1:203:GLY:O	1:A1:207:LEU:HB2	2.18	0.44
1:A2:19:ASP:N	1:A2:20:PRO:HD3	2.33	0.44
1:A2:212:TRP:HA	14:A2:1616:CLA:HBB1	2.00	0.44
14:A3:801:CLA:CGD	14:A3:801:CLA:HAA2	2.47	0.44
14:A3:826:CLA:HAB	16:A3:851:BCR:H311	2.00	0.44
14:A3:842:CLA:H192	8:J3:22:THR:HG22	1.99	0.44
1:A3:86:TRP:HE1	14:A3:808:CLA:HBA1	1.83	0.44
1:A4:212:TRP:CZ3	1:A4:215:HIS:CD2	3.06	0.44
1:A4:399:TRP:CH2	1:A4:740:ILE:HG12	2.53	0.44
1:A5:226:LEU:HD22	1:A5:231:VAL:HG21	1.99	0.44
1:A6:142:GLY:HA2	1:A6:145:GLN:HE21	1.83	0.44
1:A6:346:GLU:HA	1:A6:349:THR:HG22	2.00	0.44
2:B1:233:ALA:HB1	14:B1:817:CLA:CED	2.48	0.44
2:B1:515:PHE:HD2	14:B1:838:CLA:OBD	2.00	0.44
2:B2:207:GLY:C	14:B2:813:CLA:HMD1	2.38	0.44
2:B2:440:TYR:CE1	2:B2:524:LEU:HB3	2.52	0.44
2:B2:574:CYS:O	2:B2:575:ASP:HB2	2.16	0.44
2:B2:593:ILE:O	2:B2:597:THR:HG23	2.18	0.44
2:B2:634:SER:O	2:B2:638:ILE:HB	2.17	0.44
14:B2:817:CLA:H62	14:B2:817:CLA:H41	1.76	0.44
2:B2:173:ARG:HE	14:B2:823:CLA:HMD1	1.80	0.44
2:B3:480:LEU:C	2:B3:482:SER:N	2.70	0.44
2:B4:723:TYR:CE2	14:B4:803:CLA:HED1	2.52	0.44
14:B4:811:CLA:H102	14:B4:829:CLA:H193	1.99	0.44
14:B4:832:CLA:HBA2	14:B4:832:CLA:H3A	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B5:1806:CLA:HMB2	16:M5:101:BCR:HC42	1.99	0.44
14:L4:205:CLA:C9	14:B5:1812:CLA:H101	2.46	0.44
2:B5:181:LEU:HD21	14:B5:1815:CLA:H12	2.00	0.44
2:B6:577:SER:N	2:B6:580:ASP:OD2	2.42	0.44
2:B6:654:TRP:CD1	14:B6:802:CLA:H41	2.53	0.44
6:F6:76:TRP:CZ3	14:F6:202:CLA:CBA	2.98	0.44
10:L3:52:MET:HE1	14:L3:203:CLA:O1D	2.18	0.44
11:M3:5:ASP:HB3	11:M3:9:TYR:CE1	2.52	0.44
14:A2:1630:CLA:H62	14:A2:1630:CLA:H41	1.81	0.44
14:A2:1643:CLA:O1A	14:A2:1643:CLA:H2	2.18	0.44
1:A3:219:VAL:C	1:A3:222:PRO:HD2	2.38	0.44
1:A4:161:THR:HG22	16:A4:845:BCR:HC32	2.00	0.44
1:A4:293:TRP:O	1:A4:296:ASP:HB2	2.18	0.44
1:A5:683:TRP:CG	14:A5:801:CLA:HMA2	2.53	0.44
1:A5:654:LEU:HD11	14:A5:801:CLA:H72	1.99	0.44
1:A6:161:THR:HG22	16:A6:1644:BCR:HC32	2.00	0.44
14:A6:1626:CLA:H51	14:A6:1636:CLA:H43	2.00	0.44
14:A6:1640:CLA:H192	8:J6:22:THR:HG22	1.99	0.44
2:B1:480:LEU:C	2:B1:482:SER:N	2.71	0.44
2:B1:425:LEU:HG	14:B1:840:CLA:HBB1	1.99	0.44
14:B1:808:CLA:H91	19:B1:850:LMG:H401	2.00	0.44
14:B2:829:CLA:HBA2	14:B2:829:CLA:H3A	1.58	0.44
2:B3:256:PHE:HB2	14:B3:1818:CLA:O1D	2.18	0.44
2:B4:229:TRP:CZ3	14:B4:818:CLA:C3B	3.01	0.44
14:B4:807:CLA:H3A	14:B4:807:CLA:HBA1	1.83	0.44
2:B4:514:LEU:HD12	14:B4:828:CLA:HMC1	1.99	0.44
2:B5:599:TYR:CZ	14:B5:1839:CLA:HBC2	2.53	0.44
2:B6:573:THR:O	2:B6:576:ILE:HB	2.17	0.44
14:B6:810:CLA:CED	14:B6:810:CLA:H43	2.48	0.44
6:F3:60:ALA:O	6:F3:65:ILE:HG12	2.18	0.44
14:B5:1842:CLA:H18	16:I5:101:BCR:H362	2.00	0.44
8:J2:15:ALA:O	8:J2:19:MET:HB2	2.18	0.44
8:J4:28:GLU:HG3	14:J4:101:CLA:C1B	2.48	0.44
10:L1:59:ILE:HD11	10:L1:135:ALA:CB	2.47	0.44
11:M3:15:ALA:HB1	16:M3:1602:BCR:H17C	1.99	0.44
1:A1:477:ASP:N	1:A1:477:ASP:OD1	2.51	0.44
1:A1:90:MET:HE1	14:A1:807:CLA:HAA2	2.00	0.44
14:A2:1633:CLA:HMB2	14:A2:1634:CLA:C2D	2.48	0.44
1:A3:146:LEU:HD13	1:A3:380:TYR:CE2	2.53	0.44
1:A4:90:MET:HE2	14:A4:827:CLA:HED1	2.00	0.44
14:A5:835:CLA:H3A	14:A5:835:CLA:HBA2	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:271:ASP:HB3	14:B1:818:CLA:CMA	2.48	0.44
2:B1:349:SER:HB3	14:B1:826:CLA:C3D	2.48	0.44
2:B1:296:ILE:HG12	14:B1:822:CLA:OBD	2.15	0.44
2:B1:173:ARG:CB	14:B1:825:CLA:HMD1	2.40	0.44
2:B3:267:LEU:CD2	14:B3:1819:CLA:HBA1	2.48	0.44
14:B3:1830:CLA:H12	16:B3:1846:BCR:H393	2.00	0.44
2:B3:222:ALA:N	2:B3:223:PRO:CD	2.81	0.44
2:B4:337:LEU:HD23	2:B4:392:HIS:CE1	2.53	0.44
2:B4:664:ALA:CB	14:B4:805:CLA:CBB	2.95	0.44
14:B5:1818:CLA:H3A	14:B5:1818:CLA:HBA2	1.75	0.44
2:B5:376:THR:HG23	2:B5:597:THR:HG21	1.99	0.44
6:F2:60:ALA:O	6:F2:65:ILE:HG12	2.18	0.44
14:B2:803:CLA:H122	16:I2:101:BCR:H281	1.99	0.44
8:J6:11:ALA:N	8:J6:12:PRO:HD2	2.33	0.44
10:L4:62:TRP:CZ3	14:L4:201:CLA:H43	2.53	0.44
10:L5:53:ALA:HB3	14:L5:205:CLA:HED3	1.93	0.44
11:M1:26:SER:HB2	14:M1:1201:CLA:O2A	2.18	0.44
12:X6:9:TYR:O	12:X6:10:ALA:CB	2.65	0.44
1:A2:92:PHE:CE2	14:A2:1609:CLA:CHD	3.01	0.43
1:A3:156:PHE:CE2	14:A3:816:CLA:HAA2	2.53	0.43
1:A3:224:ASN:O	1:A3:228:ASP:CG	2.57	0.43
1:A3:360:LEU:HD13	14:A3:830:CLA:HBB1	2.00	0.43
1:A3:475:PHE:HA	1:A3:480:ILE:O	2.17	0.43
1:A3:744:TRP:HB2	14:A3:828:CLA:HBB1	1.99	0.43
1:A4:296:ASP:HB3	14:A4:817:CLA:HMA1	1.99	0.43
2:B1:442:HIS:HA	14:B1:834:CLA:C4C	2.48	0.43
2:B1:582:PHE:CD2	2:B1:583:TYR:N	2.86	0.43
2:B1:656:PHE:HZ	14:B1:804:CLA:C1D	2.31	0.43
2:B2:554:PRO:HD2	3:C2:61:PHE:CE1	2.52	0.43
2:B2:688:HIS:HE1	2:B2:697:VAL:O	2.01	0.43
14:B2:808:CLA:H201	7:I2:23:PRO:HB3	1.99	0.43
2:B3:42:TYR:CD2	2:B3:167:PHE:HB3	2.53	0.43
14:B3:1808:CLA:H143	14:B3:1830:CLA:CBB	2.48	0.43
2:B3:342:ALA:HB2	16:B3:1849:BCR:H372	2.00	0.43
2:B3:347:ILE:O	2:B3:351:VAL:HG23	2.18	0.43
2:B4:236:PRO:O	2:B4:250:GLY:HA3	2.18	0.43
14:B5:1811:CLA:HMB3	14:B5:1812:CLA:CHC	2.47	0.43
2:B6:439:LEU:HD22	2:B6:456:ILE:HG21	1.98	0.43
2:B6:456:ILE:HG22	2:B6:458:ILE:HD11	2.00	0.43
2:B6:24:ILE:HG22	14:B6:829:CLA:C4	2.48	0.43
6:F2:73:ILE:HG23	14:F2:202:CLA:HAA1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F2:78:GLY:HA3	16:F2:203:BCR:HC31	2.00	0.43
6:F6:20:ALA:O	6:F6:21:ALA:C	2.56	0.43
6:F6:63:PHE:C	6:F6:66:PRO:HD2	2.38	0.43
5:E5:39:ARG:CZ	13:P5:81:TYR:OH	2.65	0.43
1:A1:204:LEU:HD11	14:A1:828:CLA:C14	2.47	0.43
1:A2:156:PHE:CZ	14:A2:1618:CLA:HED2	2.53	0.43
1:A5:75:ALA:HB1	14:A5:805:CLA:HBB1	1.98	0.43
2:B1:217:HIS:CG	2:B1:218:PRO:HD2	2.53	0.43
2:B1:234:GLN:O	2:B1:236:PRO:HD3	2.18	0.43
2:B1:667:PHE:HB2	14:B1:806:CLA:HMC3	2.00	0.43
16:B1:844:BCR:C38	16:B1:844:BCR:H23C	2.47	0.43
14:B1:853:CLA:H3A	14:B1:853:CLA:HBA1	1.81	0.43
2:B2:493:PRO:HG3	14:B2:835:CLA:C2D	2.48	0.43
2:B2:616:ASN:HD22	2:B2:616:ASN:N	2.15	0.43
2:B3:166:TRP:CH2	14:B3:1813:CLA:HMA1	2.47	0.43
2:B3:493:PRO:CG	14:B3:1838:CLA:C3D	2.96	0.43
2:B4:691:THR:O	2:B4:695:ASN:OD1	2.36	0.43
1:A4:470:ARG:HD2	2:B4:94:GLN:O	2.18	0.43
2:B5:157:GLN:HG3	14:B5:1801:CLA:C7	2.48	0.43
2:B5:672:SER:O	15:B5:1844:PQN:H9	2.18	0.43
2:B5:90:ILE:HG21	2:B5:95:PHE:CZ	2.53	0.43
2:B6:340:HIS:CD2	14:B6:824:CLA:CAA	2.88	0.43
2:B6:713:LEU:CD1	19:B6:848:LMG:H342	2.48	0.43
5:E3:16:TRP:HA	5:E3:19:GLU:OE2	2.18	0.43
8:J1:15:ALA:O	8:J1:19:MET:HB2	2.18	0.43
10:L5:6:LYS:O	10:L5:18:SER:N	2.43	0.43
10:L5:93:LEU:O	10:L5:117:TRP:NE1	2.49	0.43
14:L6:203:CLA:H41	14:L6:203:CLA:H62	1.69	0.43
14:M3:1601:CLA:HBA2	14:M3:1601:CLA:H3A	1.73	0.43
1:A1:303:ALA:HB2	14:A1:817:CLA:CBB	2.48	0.43
1:A1:75:ALA:HB1	14:A1:804:CLA:HBB1	1.99	0.43
1:A1:199:HIS:CE1	14:A1:812:CLA:HMC2	2.53	0.43
1:A3:116:VAL:O	14:A3:809:CLA:HED2	2.19	0.43
1:A4:193:VAL:HG23	1:A4:194:GLU:OE2	2.17	0.43
14:A4:804:CLA:HMC3	14:A4:829:CLA:HMA1	2.00	0.43
16:A5:850:BCR:H402	14:B5:1802:CLA:C14	2.48	0.43
1:A6:375:TYR:OH	14:A6:1636:CLA:HBC3	2.18	0.43
2:B1:195:HIS:O	2:B1:206:VAL:HG11	2.18	0.43
2:B1:45:ILE:CD1	14:B1:807:CLA:CMC	2.95	0.43
14:B1:808:CLA:H143	14:B1:829:CLA:CBB	2.48	0.43
2:B2:372:ALA:HA	2:B2:600:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:535:THR:HB	2:B2:588:TRP:CZ3	2.52	0.43
14:B2:826:CLA:CGA	14:B2:826:CLA:H3A	2.48	0.43
2:B3:554:PRO:HD2	3:C3:61:PHE:CE1	2.53	0.43
2:B4:390:PHE:CD1	2:B4:540:LEU:HD13	2.53	0.43
2:B4:706:LEU:HD21	15:B4:844:PQN:H151	2.00	0.43
14:B4:822:CLA:HBB1	16:B4:845:BCR:H14C	2.00	0.43
16:B4:846:BCR:H23C	16:B4:846:BCR:C38	2.48	0.43
2:B6:430:LEU:HB3	14:B6:832:CLA:CED	2.46	0.43
3:C2:33:CYS:SG	3:C2:34:LYS:N	2.92	0.43
3:C6:28:VAL:HG12	4:D6:109:ARG:CB	2.47	0.43
5:E3:59:ASN:OD1	5:E3:59:ASN:N	2.51	0.43
6:F2:37:ARG:O	6:F2:40:GLN:HG2	2.17	0.43
14:L3:202:CLA:HBA2	14:L3:202:CLA:H3A	1.75	0.43
1:A4:36:ARG:NH1	13:P4:71:GLU:HG3	2.33	0.43
12:X1:9:TYR:O	12:X1:10:ALA:CB	2.67	0.43
1:A2:746:PHE:CD2	14:A2:1602:CLA:HMD1	2.53	0.43
14:A2:1641:CLA:HBB1	14:A2:1642:CLA:HMD1	2.00	0.43
1:A3:193:VAL:HG23	1:A3:325:LEU:HD12	2.00	0.43
1:A3:726:GLN:O	1:A3:730:VAL:HG23	2.18	0.43
14:A4:842:CLA:H3A	14:A4:842:CLA:HBA2	1.80	0.43
14:A4:825:CLA:HAB	16:A4:848:BCR:H311	1.99	0.43
14:B4:852:CLA:CMC	1:A6:332:HIS:CD2	3.01	0.43
2:B1:229:TRP:HB3	14:B1:817:CLA:H3A	2.00	0.43
2:B1:664:ALA:HB3	14:B1:806:CLA:HBB2	2.00	0.43
2:B2:694:ALA:O	2:B2:697:VAL:HG22	2.18	0.43
2:B3:470:HIS:HB3	14:B3:1836:CLA:HED1	1.99	0.43
2:B3:481:LEU:HA	2:B3:489:SER:OG	2.18	0.43
2:B4:494:ASN:ND2	14:B4:837:CLA:CED	2.81	0.43
2:B4:375:TYR:CE2	2:B4:600:TRP:CD1	3.06	0.43
2:B4:657:LEU:HB3	14:B4:801:CLA:O2A	2.18	0.43
2:B4:91:TRP:N	14:B4:811:CLA:O1D	2.36	0.43
2:B5:360:PRO:HG3	14:B5:1820:CLA:CBA	2.47	0.43
2:B5:182:PHE:CE1	14:B5:1826:CLA:HED2	2.53	0.43
14:B6:819:CLA:CMD	14:B6:821:CLA:HBB1	2.48	0.43
10:L2:79:LEU:HD22	10:L2:136:PHE:CG	2.53	0.43
14:A6:1631:CLA:HMB2	14:L6:202:CLA:C2D	2.48	0.43
12:X2:9:TYR:O	12:X2:10:ALA:CB	2.66	0.43
1:A1:718:GLN:HA	1:A1:719:PRO:HD3	1.90	0.43
1:A2:189:TRP:HZ3	14:A2:1615:CLA:HMD3	1.84	0.43
1:A2:207:LEU:HD22	16:A2:1648:BCR:H361	1.99	0.43
1:A3:216:GLN:NE2	1:A3:297:THR:OG1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:366:LEU:HD11	14:A3:819:CLA:C5	2.48	0.43
1:A3:403:PHE:HB3	14:A3:806:CLA:H112	2.01	0.43
1:A3:464:THR:HG22	1:A3:468:PHE:CE1	2.53	0.43
1:A3:497:ALA:N	1:A3:498:PRO:CD	2.81	0.43
14:A3:826:CLA:H51	14:A3:837:CLA:H43	2.01	0.43
14:A3:831:CLA:HMB2	14:A3:832:CLA:C2D	2.49	0.43
1:A4:237:PRO:CB	1:A4:248:LEU:HD21	2.48	0.43
1:A5:565:LEU:HD11	1:A5:583:ARG:HB3	2.00	0.43
2:B1:227:GLY:O	14:B1:817:CLA:H11	2.18	0.43
2:B2:430:LEU:O	2:B2:434:PHE:CD1	2.71	0.43
14:B2:805:CLA:H91	19:B2:848:LMG:H401	2.01	0.43
2:B3:65:PHE:CD2	14:B3:1809:CLA:C4C	3.01	0.43
1:A3:651:ARG:HG3	2:B3:638:ILE:CG2	2.48	0.43
2:B3:718:HIS:CE1	14:B3:1843:CLA:C4D	3.01	0.43
14:B4:808:CLA:H41	14:B4:808:CLA:H61	1.70	0.43
2:B4:529:ILE:HG21	14:B4:839:CLA:CAB	2.49	0.43
2:B5:337:LEU:HB2	14:B5:1807:CLA:HMD3	1.99	0.43
2:B6:182:PHE:HD1	14:B6:819:CLA:HBB2	1.84	0.43
2:B6:354:HIS:CE1	14:B6:826:CLA:NB	2.86	0.43
2:B6:564:PRO:O	2:B6:565:CYS:CB	2.66	0.43
3:C2:20:CYS:SG	18:C2:101:SF4:S4	3.13	0.43
14:B1:834:CLA:H122	6:F1:69:LEU:HD11	2.01	0.43
14:B2:806:CLA:C4	7:I2:14:PHE:CZ	3.01	0.43
7:I4:10:LEU:HD12	7:I4:10:LEU:HA	1.87	0.43
1:A5:118:TRP:HB3	16:J5:104:BCR:HC21	1.99	0.43
14:L1:205:CLA:CBA	16:L1:209:BCR:H363	2.40	0.43
16:L2:208:BCR:C8	16:L2:208:BCR:H331	2.47	0.43
10:L3:52:MET:CB	14:L3:203:CLA:HMA2	2.48	0.43
10:L5:37:TYR:O	10:L5:38:ARG:O	2.37	0.43
11:M3:12:LEU:HD22	16:M3:1602:BCR:C20	2.48	0.43
13:P3:62:GLN:HB2	13:P3:76:LEU:HD12	2.01	0.43
1:A1:431:ASP:O	1:A1:435:ARG:HG3	2.19	0.43
1:A1:352:TRP:HZ3	14:A1:824:CLA:H112	1.84	0.43
1:A2:203:GLY:O	1:A2:207:LEU:HB2	2.18	0.43
1:A2:363:MET:CE	14:A2:1631:CLA:HBC3	2.47	0.43
1:A3:385:THR:HG23	1:A3:523:LYS:HB2	2.00	0.43
1:A3:212:TRP:N	14:A3:814:CLA:HBB1	2.33	0.43
14:A3:834:CLA:CGA	10:L3:62:TRP:NE1	2.82	0.43
1:A4:189:TRP:CZ2	14:A4:812:CLA:HAC2	2.53	0.43
14:A6:1623:CLA:HBA2	14:A6:1623:CLA:H3A	1.87	0.43
14:A6:1640:CLA:H172	8:J6:19:MET:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:526:HIS:HA	2:B1:529:ILE:HD12	2.00	0.43
2:B1:70:GLN:NE2	14:B1:809:CLA:O1D	2.46	0.43
2:B2:60:VAL:HB	2:B2:141:LEU:HD13	2.01	0.43
14:B2:809:CLA:H162	10:L3:56:TYR:CZ	2.51	0.43
2:B2:427:TRP:CE2	14:B2:830:CLA:CBB	3.02	0.43
2:B3:462:PHE:HB3	14:B3:1839:CLA:H42	2.01	0.43
2:B4:539:ILE:HG12	14:B4:802:CLA:HMD1	1.99	0.43
2:B4:664:ALA:HB3	14:B4:805:CLA:CBB	2.46	0.43
2:B6:195:HIS:O	2:B6:206:VAL:HG11	2.16	0.43
2:B6:376:THR:HG23	2:B6:597:THR:CG2	2.48	0.43
4:D4:118:SER:HB3	5:E4:34:TYR:OH	2.18	0.43
14:L1:205:CLA:H111	7:I3:25:VAL:HG13	2.01	0.43
16:L1:209:BCR:C39	10:L3:83:ILE:HD11	2.48	0.43
10:L4:48:LEU:HD11	10:L5:125:PHE:HD2	1.83	0.43
10:L5:62:TRP:CD1	14:L5:203:CLA:O1A	2.72	0.43
10:L5:96:TYR:O	10:L5:100:SER:OG	2.37	0.43
14:B3:1801:CLA:CGA	14:M3:1601:CLA:HAA2	2.48	0.43
13:P6:62:GLN:HB2	13:P6:76:LEU:HD12	2.01	0.43
1:A1:296:ASP:HB3	14:A1:817:CLA:HMA1	2.01	0.43
14:A1:840:CLA:H3A	14:A1:840:CLA:HBA2	1.81	0.43
1:A4:203:GLY:HA2	14:A4:819:CLA:CBC	2.41	0.43
1:A5:203:GLY:O	1:A5:207:LEU:HB2	2.19	0.43
1:A5:300:HIS:HE2	14:A5:819:CLA:C2B	2.32	0.43
1:A5:161:THR:HG22	16:A5:846:BCR:HC32	2.00	0.43
1:A6:75:ALA:HB1	14:A6:1605:CLA:HBB1	2.00	0.43
1:A6:436:HIS:CD2	1:A6:440:ILE:HG13	2.54	0.43
1:A6:388:PRO:HA	1:A6:751:ILE:HG21	2.01	0.43
2:B1:466:ILE:HD11	14:B1:838:CLA:C1	2.48	0.43
2:B1:656:PHE:HZ	14:B1:804:CLA:CHD	2.31	0.43
14:B1:854:CLA:H43	14:B1:854:CLA:CED	2.48	0.43
2:B3:622:LEU:HD13	14:B3:1804:CLA:CMA	2.49	0.43
10:L1:148:ILE:HG23	14:B3:1812:CLA:CGA	2.48	0.43
2:B3:222:ALA:HB3	2:B3:223:PRO:HD3	2.01	0.43
2:B3:466:ILE:HG22	2:B3:470:HIS:CE1	2.54	0.43
2:B3:368:HIS:CE1	2:B3:608:TRP:CD1	3.07	0.43
2:B3:625:TRP:O	2:B3:629:TYR:HB3	2.19	0.43
2:B5:381:ILE:HD12	14:B5:1830:CLA:CBB	2.49	0.43
2:B5:529:ILE:HG21	14:B5:1839:CLA:CAB	2.49	0.43
2:B6:222:ALA:HB3	2:B6:223:PRO:HD3	2.01	0.43
2:B6:554:PRO:HD2	3:C6:61:PHE:CZ	2.53	0.43
2:B6:682:GLU:HG2	3:C6:80:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B6:699:TRP:HD1	2:B6:699:TRP:O	2.01	0.43
5:E4:37:ILE:CD1	13:P4:41:ARG:HD2	2.46	0.43
6:F5:103:VAL:HB	6:F5:104:PRO:HD3	1.99	0.43
7:I2:9:PHE:CE1	7:I2:10:LEU:HD12	2.54	0.43
8:J3:31:ARG:CZ	14:J3:101:CLA:HED2	2.49	0.43
8:J4:27:ILE:HG22	16:J4:104:BCR:H343	1.98	0.43
8:J6:12:PRO:HG3	14:J6:1101:CLA:ND	2.34	0.43
10:L1:71:SER:OG	10:L1:73:VAL:HG22	2.19	0.43
10:L3:50:VAL:HA	14:L3:204:CLA:O1D	2.18	0.43
14:A3:834:CLA:O1D	10:L3:67:PRO:HB3	2.19	0.43
14:L4:203:CLA:H42	16:L4:208:BCR:H12C	2.00	0.43
2:B4:693:LEU:CD1	14:L4:204:CLA:H11	2.49	0.43
10:L4:46:ARG:O	10:L4:50:VAL:HG23	2.18	0.43
13:P5:62:GLN:HB2	13:P5:76:LEU:HD12	2.01	0.43
1:A1:436:HIS:CE1	1:A1:440:ILE:HD11	2.53	0.43
1:A1:444:LEU:HB2	14:A1:836:CLA:CBB	2.48	0.43
1:A1:459:TYR:CE1	1:A1:537:MET:HB3	2.54	0.43
1:A1:300:HIS:HB2	14:A1:817:CLA:C1B	2.48	0.43
1:A2:142:GLY:HA2	1:A2:145:GLN:HE21	1.84	0.43
1:A2:89:GLY:CA	14:A2:1609:CLA:HMC3	2.49	0.43
1:A2:200:HIS:CE1	14:A2:1627:CLA:H52	2.53	0.43
1:A3:148:ARG:NH2	1:A3:227:LEU:HB3	2.34	0.43
1:A3:336:PHE:CB	17:A3:854:LHG:HC41	2.46	0.43
1:A4:576:PHE:C	1:A4:725:ILE:HD11	2.39	0.43
14:A4:820:CLA:HBB1	14:A4:820:CLA:HMB1	2.01	0.43
14:A4:841:CLA:HHC	14:A4:841:CLA:HBB1	2.00	0.43
1:A5:744:TRP:CE3	16:A5:850:BCR:H313	2.53	0.43
1:A6:302:LEU:HD21	14:A6:1617:CLA:C2B	2.48	0.43
1:A6:52:HIS:HB2	17:A6:1649:LHG:H102	2.00	0.43
1:A6:77:PHE:CE2	14:A6:1610:CLA:HBB1	2.54	0.43
2:B1:122:TRP:HZ2	14:B1:814:CLA:C19	2.16	0.43
2:B1:587:PHE:HB2	14:B1:802:CLA:CAC	2.49	0.43
2:B2:214:THR:O	14:B2:814:CLA:HED1	2.19	0.43
14:B3:1829:CLA:CGA	14:B3:1829:CLA:H3A	2.49	0.43
2:B3:351:VAL:HG21	14:B3:1830:CLA:HHD	2.00	0.43
2:B4:194:ILE:HA	2:B4:198:ILE:HD12	2.01	0.43
3:C5:5:LYS:C	3:C5:6:ILE:HD12	2.39	0.43
14:B1:854:CLA:HBB2	7:I1:19:CYS:HB3	2.01	0.43
7:I1:30:LEU:HD11	16:I1:103:BCR:H312	2.00	0.43
10:L3:64:LYS:HB2	14:L3:205:CLA:HMB3	2.01	0.43
14:L5:202:CLA:H3A	14:L5:202:CLA:HBA2	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:399:TRP:NE1	14:A1:827:CLA:HAB	2.32	0.43
1:A1:207:LEU:CD2	16:A1:843:BCR:H361	2.40	0.43
1:A1:86:TRP:O	1:A1:90:MET:HG2	2.18	0.43
1:A2:156:PHE:CE2	14:A2:1618:CLA:HED2	2.54	0.43
1:A2:293:TRP:O	1:A2:296:ASP:HB2	2.18	0.43
1:A3:161:THR:HG22	16:A3:848:BCR:HC32	2.01	0.43
1:A4:283:GLY:O	1:A4:507:ALA:HB3	2.19	0.43
1:A4:686:SER:HB3	1:A4:734:HIS:CB	2.46	0.43
14:A4:853:CLA:HMD2	10:L4:21:ILE:CD1	2.48	0.43
1:A5:375:TYR:C	1:A5:375:TYR:CD1	2.92	0.43
1:A5:79:HIS:CE1	14:A5:805:CLA:HMA2	2.54	0.43
14:A5:828:CLA:H62	14:A5:828:CLA:H41	1.79	0.43
1:A6:409:ALA:HA	16:A6:1647:BCR:HC41	2.00	0.43
2:B1:220:GLY:HA3	14:B1:816:CLA:HMD1	2.01	0.43
2:B1:525:VAL:CG1	14:B1:804:CLA:C14	2.91	0.43
2:B1:685:VAL:HG11	3:C1:80:TYR:CD1	2.54	0.43
14:B1:805:CLA:H61	14:B1:805:CLA:H41	1.64	0.43
2:B1:216:PRO:HG2	14:B1:816:CLA:C1D	2.49	0.43
1:A2:651:ARG:HB2	2:B2:638:ILE:HG23	2.01	0.43
2:B3:642:ASN:HB2	2:B3:643:PRO:HD2	2.00	0.43
2:B4:28:HIS:HE1	14:B4:808:CLA:HED1	1.83	0.43
2:B4:642:ASN:HB2	2:B4:643:PRO:HD2	2.01	0.43
14:B4:812:CLA:H43	14:B4:812:CLA:CED	2.49	0.43
2:B4:466:ILE:CD1	14:B4:839:CLA:O2A	2.64	0.43
2:B5:313:LYS:O	2:B5:314:VAL:CG2	2.60	0.43
2:B5:361:TYR:O	2:B5:364:ILE:HG22	2.18	0.43
3:C2:54:GLU:HG2	3:C2:62:LEU:HD13	2.00	0.43
3:C5:74:ARG:NH2	4:D5:25:GLU:OE1	2.52	0.43
6:F2:69:LEU:CA	14:F2:204:CLA:HBB2	2.49	0.43
8:J1:21:ILE:O	14:J1:101:CLA:HBB2	2.19	0.43
10:L1:52:MET:HE2	14:L1:205:CLA:H2A	2.01	0.43
10:L2:125:PHE:CD2	10:L3:48:LEU:HD11	2.54	0.43
14:A1:805:CLA:H62	14:A1:805:CLA:H41	1.81	0.43
14:A1:808:CLA:CBB	14:B1:834:CLA:HMD2	2.48	0.43
14:A1:838:CLA:O1A	14:A1:838:CLA:H2	2.19	0.43
1:A3:47:TRP:CZ3	1:A3:51:LEU:HD12	2.53	0.43
14:A4:841:CLA:H151	10:L4:85:LEU:CD2	2.48	0.43
16:A4:849:BCR:H402	14:B4:802:CLA:C14	2.48	0.43
1:A5:117:VAL:HG12	1:A5:118:TRP:O	2.19	0.43
1:A5:501:THR:C	1:A5:503:PRO:HD3	2.39	0.43
1:A6:275:TYR:CE2	14:A6:1615:CLA:HMD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A6:1626:CLA:HAB	16:A6:1647:BCR:H311	2.00	0.43
2:B2:189:TRP:HA	14:B2:813:CLA:HBB1	2.01	0.43
2:B2:264:THR:HG22	2:B2:363:PHE:CZ	2.54	0.43
14:B2:809:CLA:H43	14:B2:809:CLA:CED	2.49	0.43
2:B2:24:ILE:HG22	14:B2:828:CLA:C4	2.49	0.43
2:B3:166:TRP:CE2	14:B3:1813:CLA:HMA2	2.54	0.43
2:B3:73:PHE:O	2:B3:77:VAL:HG23	2.19	0.43
2:B4:196:VAL:HG11	14:B4:816:CLA:O2D	2.19	0.43
14:B6:820:CLA:HBA2	14:B6:820:CLA:H3A	1.70	0.43
3:C2:17:VAL:HG21	3:C2:27:MET:SD	2.59	0.43
3:C5:2:HIS:NE2	3:C5:68:LEU:HD22	2.34	0.43
6:F4:70:PHE:HE1	16:F4:201:BCR:C9	2.25	0.43
14:B2:808:CLA:C19	7:I2:26:VAL:HG21	2.45	0.43
7:I5:9:PHE:C	7:I5:11:PRO:HD2	2.39	0.43
8:J1:39:HIS:HE1	14:J1:102:CLA:NA	2.17	0.43
14:A2:1601:CLA:CAC	14:L2:206:CLA:H151	2.48	0.43
10:L3:61:PRO:HA	14:L3:205:CLA:HMB3	2.01	0.43
10:L4:40:GLY:HA2	10:L5:115:GLU:OE2	2.18	0.43
10:L5:64:LYS:HB2	14:L5:206:CLA:CMB	2.48	0.43
10:L5:66:GLY:HA2	14:L5:203:CLA:HAA1	2.01	0.43
12:X1:26:VAL:HG12	14:X1:1701:CLA:CED	2.49	0.43
1:A1:501:THR:C	1:A1:503:PRO:HD3	2.39	0.42
16:A1:847:BCR:H402	14:B1:802:CLA:C14	2.49	0.42
14:A2:1608:CLA:H41	14:A2:1608:CLA:H62	1.78	0.42
1:A2:212:TRP:N	14:A2:1616:CLA:HBB1	2.34	0.42
1:A4:74:SER:OG	1:A4:180:TYR:HB2	2.19	0.42
1:A5:104:LEU:CD1	1:A5:153:THR:HA	2.49	0.42
1:A5:293:TRP:O	1:A5:296:ASP:HB2	2.18	0.42
1:A6:90:MET:CE	14:A6:1628:CLA:HED1	2.49	0.42
14:A6:1603:CLA:C14	16:A6:1648:BCR:H402	2.49	0.42
1:A6:592:TRP:NE1	14:A6:1630:CLA:HMD1	2.33	0.42
2:B1:229:TRP:CA	14:B1:817:CLA:HBA2	2.47	0.42
2:B2:523:PHE:HE1	14:B2:837:CLA:C2D	2.33	0.42
2:B3:487:ILE:C	14:B3:1837:CLA:HMD3	2.39	0.42
2:B4:58:LEU:O	14:B4:809:CLA:HBB2	2.19	0.42
2:B5:118:GLY:O	14:B5:1830:CLA:HED1	2.19	0.42
2:B5:264:THR:HG22	2:B5:363:PHE:CZ	2.53	0.42
2:B5:500:LEU:O	2:B5:504:LEU:HG	2.19	0.42
2:B5:685:VAL:HG11	3:C5:80:TYR:CG	2.54	0.42
2:B5:685:VAL:HG21	3:C5:80:TYR:CE1	2.54	0.42
1:A2:438:ASP:OD1	4:D2:14:THR:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:435:ARG:NH1	4:D3:12:GLY:O	2.48	0.42
4:D6:112:VAL:O	4:D6:113:ASN:HB2	2.19	0.42
14:B2:808:CLA:H201	7:I2:23:PRO:CB	2.49	0.42
7:I3:20:TRP:C	7:I3:23:PRO:HD2	2.40	0.42
8:J6:19:MET:HB3	14:J6:1101:CLA:H142	2.01	0.42
10:L1:145:VAL:O	10:L1:148:ILE:HB	2.19	0.42
10:L2:110:PRO:HA	10:L2:113:THR:HG23	2.00	0.42
11:M3:15:ALA:CB	16:M3:1602:BCR:H17C	2.49	0.42
1:A2:40:ARG:CA	13:P2:60:SER:HB2	2.49	0.42
1:A1:363:MET:CE	14:A1:805:CLA:HBB2	2.49	0.42
14:A1:822:CLA:HBA2	14:A1:822:CLA:H3A	1.87	0.42
14:A1:825:CLA:H51	14:A1:834:CLA:H43	2.01	0.42
1:A1:447:VAL:CG2	14:A1:836:CLA:HMC3	2.48	0.42
1:A2:440:ILE:HG12	14:A2:1633:CLA:C4B	2.49	0.42
1:A3:28:TRP:CZ2	14:A3:804:CLA:H11	2.54	0.42
1:A4:120:ILE:O	1:A4:122:GLY:N	2.52	0.42
1:A4:257:ASP:O	1:A4:258:TRP:HB2	2.19	0.42
14:A4:819:CLA:H3A	14:A4:819:CLA:HBA2	1.88	0.42
1:A4:726:GLN:NE2	17:A4:850:LHG:HC81	2.34	0.42
1:A5:468:PHE:CD2	2:B5:95:PHE:HA	2.54	0.42
1:A6:115:GLN:HE22	14:A6:1608:CLA:C4B	2.31	0.42
1:A6:654:LEU:HD11	14:A6:1602:CLA:H72	2.00	0.42
2:B1:45:ILE:HD11	14:B1:807:CLA:HMC2	2.01	0.42
2:B2:419:GLU:CD	2:B2:419:GLU:H	2.22	0.42
2:B2:658:PHE:CE2	2:B2:725:LEU:HD13	2.54	0.42
2:B2:144:LEU:CD2	14:B2:813:CLA:H152	2.49	0.42
2:B2:25:ALA:HA	14:B2:828:CLA:H42	2.02	0.42
14:B2:837:CLA:CGA	14:B2:837:CLA:C1A	2.97	0.42
14:B3:1801:CLA:HBA1	14:B3:1801:CLA:H3A	1.79	0.42
2:B3:192:HIS:HB2	14:B3:1816:CLA:C1C	2.50	0.42
2:B5:598:PHE:CE1	14:B5:1803:CLA:HED2	2.54	0.42
2:B6:100:VAL:HG13	2:B6:111:PRO:HG3	2.01	0.42
14:A6:1639:CLA:HMD1	14:B6:803:CLA:HBB1	2.01	0.42
3:C5:42:PRO:HG2	3:C5:43:ARG:HG3	2.01	0.42
3:C5:53:CYS:HB2	3:C5:64:ILE:HD13	2.00	0.42
4:D5:39:PHE:HE1	4:D5:67:LEU:HD11	1.82	0.42
5:E3:68:VAL:O	5:E3:69:ALA:O	2.37	0.42
1:A6:718:GLN:CD	5:E6:15:TYR:OH	2.56	0.42
2:B2:91:TRP:CD2	7:I2:11:PRO:HB2	2.54	0.42
7:I4:20:TRP:CE2	16:I4:102:BCR:HC31	2.53	0.42
7:I4:29:LEU:HD23	14:L6:206:CLA:CBC	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I5:13:ILE:O	7:I5:17:VAL:HG23	2.18	0.42
14:A1:802:CLA:HED1	8:J1:12:PRO:HA	2.00	0.42
10:L2:57:PHE:CD1	10:L2:57:PHE:C	2.92	0.42
10:L5:141:ASN:O	10:L5:144:VAL:HB	2.18	0.42
10:L5:38:ARG:NH1	14:L5:204:CLA:CHD	2.82	0.42
11:M3:17:LEU:HB3	11:M3:18:PRO:HD3	2.00	0.42
1:A1:168:MET:O	1:A1:172:MET:HB2	2.19	0.42
1:A1:220:SER:O	1:A1:224:ASN:HB2	2.18	0.42
1:A1:283:GLY:O	1:A1:507:ALA:HB3	2.19	0.42
1:A1:605:CYS:O	1:A1:609:VAL:HG23	2.19	0.42
1:A1:71:LYS:HZ1	14:A1:810:CLA:HED2	1.80	0.42
1:A2:120:ILE:O	1:A2:123:GLN:HG2	2.18	0.42
14:A2:1605:CLA:H142	8:J2:19:MET:HB3	2.01	0.42
1:A2:501:THR:C	1:A2:503:PRO:HD3	2.39	0.42
1:A2:602:MET:C	1:A2:602:MET:SD	2.98	0.42
1:A3:212:TRP:HA	14:A3:814:CLA:HBB1	2.01	0.42
1:A3:593:ASP:OD1	1:A3:728:ARG:NH1	2.52	0.42
14:A3:840:CLA:HBB1	14:A3:841:CLA:HMD1	2.00	0.42
14:A3:842:CLA:O1A	14:A3:842:CLA:H2	2.19	0.42
14:A3:842:CLA:H62	14:A3:842:CLA:H41	1.83	0.42
1:A4:682:ILE:HD11	16:A4:849:BCR:C13	2.49	0.42
14:A5:826:CLA:H51	14:A5:836:CLA:H43	2.01	0.42
2:B1:222:ALA:N	2:B1:223:PRO:CD	2.82	0.42
2:B1:706:LEU:HG	15:B1:842:PQN:O4	2.18	0.42
2:B1:499:TRP:CZ2	14:B1:836:CLA:CMA	3.02	0.42
14:B1:853:CLA:CMC	1:A2:332:HIS:CD2	3.02	0.42
2:B2:274:HIS:HE1	14:B2:815:CLA:C4D	2.32	0.42
2:B2:625:TRP:O	2:B2:629:TYR:HB3	2.19	0.42
14:B2:802:CLA:H41	14:B2:802:CLA:H61	1.66	0.42
2:B3:376:THR:HG21	2:B3:727:TYR:HE2	1.83	0.42
2:B3:65:PHE:CE2	14:B3:1809:CLA:C3C	3.02	0.42
2:B5:222:ALA:N	2:B5:223:PRO:CD	2.82	0.42
2:B6:521:GLY:HA3	2:B6:619:SER:OG	2.19	0.42
2:B6:533:LEU:HD23	2:B6:592:THR:HG21	2.01	0.42
2:B6:637:LEU:HG	2:B6:638:ILE:HD12	2.02	0.42
2:B6:690:ARG:CZ	10:L6:16:HIS:HB2	2.49	0.42
4:D3:9:LEU:HB2	4:D3:48:VAL:HB	2.01	0.42
14:J6:1102:CLA:HBA2	14:J6:1102:CLA:H3A	1.68	0.42
10:L2:68:LEU:N	10:L2:68:LEU:HD23	2.34	0.42
10:L4:43:PRO:HA	10:L4:46:ARG:HD2	2.01	0.42
10:L4:63:VAL:HG22	10:L4:75:ASN:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L5:54:HIS:O	10:L5:57:PHE:CD2	2.72	0.42
1:A3:40:ARG:HG3	13:P3:60:SER:O	2.15	0.42
1:A1:120:ILE:O	1:A1:122:GLY:N	2.53	0.42
1:A1:726:GLN:NE2	17:A1:848:LHG:HC81	2.33	0.42
14:A2:1607:CLA:HMC3	14:A2:1632:CLA:HMA1	2.00	0.42
1:A2:300:HIS:NE2	14:A2:1621:CLA:C1B	2.82	0.42
14:A2:1628:CLA:H51	14:A2:1638:CLA:H43	2.00	0.42
1:A4:24:SER:O	14:A4:810:CLA:HMA1	2.19	0.42
14:A4:825:CLA:H51	14:A4:835:CLA:H43	2.00	0.42
1:A5:622:TRP:O	1:A5:633:HIS:CD2	2.73	0.42
1:A5:677:LEU:HD11	2:B5:623:MET:CB	2.46	0.42
14:A5:805:CLA:HMC3	14:A5:830:CLA:HMA1	2.01	0.42
1:A5:447:VAL:CG2	14:A5:838:CLA:HMC3	2.49	0.42
14:A5:842:CLA:HBB1	14:A5:842:CLA:HHC	2.01	0.42
1:A6:120:ILE:O	1:A6:122:GLY:N	2.52	0.42
14:A6:1609:CLA:CBB	14:B6:833:CLA:HMD2	2.49	0.42
1:A6:660:GLN:HG2	1:A6:753:SER:HB3	2.01	0.42
2:B1:379:GLN:OE1	2:B1:379:GLN:HA	2.19	0.42
2:B1:504:LEU:HA	2:B1:507:ILE:HG22	2.01	0.42
2:B1:289:MET:HE2	14:B1:820:CLA:O1D	2.19	0.42
14:B1:820:CLA:CMD	14:B1:822:CLA:HBB1	2.48	0.42
2:B2:380:TYR:CD1	2:B2:593:ILE:HG21	2.55	0.42
14:B3:1812:CLA:H43	14:B3:1812:CLA:CED	2.48	0.42
2:B3:195:HIS:CE1	14:B3:1816:CLA:CBC	3.02	0.42
2:B3:214:THR:O	14:B3:1817:CLA:CED	2.67	0.42
2:B4:140:PHE:CE2	2:B4:144:LEU:HD11	2.53	0.42
2:B4:564:PRO:O	2:B4:565:CYS:CB	2.67	0.42
2:B4:125:THR:HG21	14:B4:820:CLA:HED1	2.01	0.42
14:B4:827:CLA:H3A	14:B4:827:CLA:HBA2	1.72	0.42
14:B5:1812:CLA:CED	14:B5:1812:CLA:H43	2.49	0.42
14:B5:1810:CLA:O1A	14:B5:1829:CLA:HBD	2.19	0.42
2:B5:434:PHE:CE2	14:B5:1802:CLA:C2	3.02	0.42
2:B6:713:LEU:HD11	19:B6:848:LMG:H342	2.01	0.42
14:B6:809:CLA:H102	14:B6:827:CLA:H193	2.00	0.42
2:B6:530:ALA:HB2	14:B6:838:CLA:HMA1	2.02	0.42
3:C1:13:CYS:SG	18:C1:102:SF4:S4	3.17	0.42
4:D5:39:PHE:CD1	4:D5:67:LEU:HD11	2.53	0.42
4:D6:95:HIS:HA	4:D6:97:LYS:N	2.34	0.42
5:E5:45:TYR:O	5:E5:46:THR:C	2.58	0.42
2:B2:91:TRP:CE3	7:I2:11:PRO:HB2	2.54	0.42
8:J5:36:LEU:HD22	16:J5:105:BCR:C21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A6:1643:BCR:H402	9:K6:65:PHE:CB	2.48	0.42
10:L3:43:PRO:HA	10:L3:46:ARG:HD2	2.01	0.42
13:P5:54:GLU:HG2	13:P5:87:LYS:HB3	2.01	0.42
1:A1:293:TRP:O	1:A1:296:ASP:HB2	2.18	0.42
1:A1:588:GLN:HA	1:A1:593:ASP:OD2	2.19	0.42
14:A2:1634:CLA:CAD	10:L2:21:ILE:HB	2.49	0.42
16:A2:1652:BCR:H362	14:B2:802:CLA:C4	2.36	0.42
1:A3:283:GLY:O	1:A3:507:ALA:HB3	2.19	0.42
14:A3:801:CLA:NA	14:B3:1803:CLA:HAB	2.35	0.42
1:A4:483:GLN:HA	1:A4:484:PRO:HD3	1.80	0.42
1:A4:709:ASN:HB3	6:F4:136:ILE:HG23	2.00	0.42
14:A4:841:CLA:HMA1	2:B4:694:ALA:HB1	2.01	0.42
1:A5:219:VAL:C	1:A5:222:PRO:HD2	2.40	0.42
1:A5:300:HIS:HB2	14:A5:818:CLA:CHB	2.49	0.42
1:A6:373:HIS:ND1	14:A6:1618:CLA:OBD	2.29	0.42
1:A6:16:VAL:HG12	1:A6:17:ASP:N	2.35	0.42
2:B1:229:TRP:CH2	14:B1:817:CLA:C7	2.97	0.42
2:B2:699:TRP:CD1	2:B2:702:LYS:HA	2.54	0.42
14:B2:819:CLA:HBB1	16:B2:842:BCR:H14C	2.01	0.42
1:A2:121:VAL:HB	14:B2:832:CLA:HMD1	2.00	0.42
2:B3:390:PHE:HB2	2:B3:540:LEU:HD22	2.00	0.42
14:A5:801:CLA:NA	14:B5:1803:CLA:HAB	2.34	0.42
14:B5:1826:CLA:H61	14:B5:1826:CLA:H41	1.76	0.42
14:B5:1837:CLA:HBA2	14:B5:1838:CLA:HMB3	2.00	0.42
2:B5:25:ALA:HB2	19:B5:1851:LMG:H121	2.00	0.42
2:B5:662:VAL:HG22	14:B5:1843:CLA:HMB3	2.02	0.42
2:B6:236:PRO:O	2:B6:250:GLY:HA3	2.18	0.42
2:B6:390:PHE:HZ	14:B6:825:CLA:HAB	1.85	0.42
5:E2:57:THR:HG23	13:P2:42:ALA:CB	2.42	0.42
8:J2:21:ILE:O	14:J2:101:CLA:HBB2	2.20	0.42
13:P1:62:GLN:HB2	13:P1:76:LEU:HD12	2.01	0.42
13:P2:54:GLU:HG2	13:P2:87:LYS:HB3	2.02	0.42
13:P3:54:GLU:HG2	13:P3:87:LYS:HB3	2.01	0.42
1:A1:212:TRP:N	14:A1:813:CLA:HBB1	2.34	0.42
1:A1:372:GLN:HG3	14:A1:825:CLA:HED2	2.02	0.42
1:A1:483:GLN:HA	1:A1:484:PRO:HD3	1.79	0.42
1:A1:489:TRP:O	1:A1:493:LEU:HG	2.19	0.42
14:A1:801:CLA:NA	14:B1:804:CLA:HAB	2.35	0.42
14:A2:1644:CLA:HBB1	14:A2:1644:CLA:HHC	2.00	0.42
1:A3:392:SER:HB3	14:A3:828:CLA:HMA1	2.02	0.42
15:A3:846:PQN:H191	15:A3:846:PQN:H212	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:332:HIS:HB3	17:A4:851:LHG:O1	2.20	0.42
1:A4:275:TYR:CE2	14:A4:814:CLA:HMD2	2.54	0.42
1:A4:196:MET:CE	14:A4:824:CLA:H142	2.50	0.42
1:A5:95:ALA:HB2	1:A5:158:LEU:HB2	2.00	0.42
1:A6:114:ALA:O	1:A6:115:GLN:O	2.38	0.42
14:A6:1601:CLA:HBA2	14:A6:1601:CLA:H3A	1.73	0.42
1:A6:682:ILE:HD11	16:A6:1648:BCR:C15	2.49	0.42
1:A6:283:GLY:O	1:A6:507:ALA:HB3	2.19	0.42
2:B1:236:PRO:O	2:B1:250:GLY:HA3	2.19	0.42
2:B1:26:MET:O	2:B1:27:ALA:C	2.57	0.42
2:B1:339:TRP:HZ3	14:B1:824:CLA:CBC	2.32	0.42
2:B1:377:HIS:HB2	14:B1:828:CLA:C1B	2.49	0.42
2:B1:654:TRP:CZ2	14:B1:801:CLA:H52	2.54	0.42
2:B1:271:ASP:CB	14:B1:818:CLA:HMA1	2.49	0.42
14:B2:823:CLA:H41	14:B2:823:CLA:H61	1.76	0.42
1:A3:691:PHE:HB2	14:B3:1802:CLA:HBC2	2.01	0.42
2:B3:494:ASN:HB3	14:B3:1838:CLA:O1D	2.19	0.42
2:B3:386:MET:HE1	16:B3:1849:BCR:H361	2.00	0.42
2:B3:480:LEU:HB3	14:B3:1836:CLA:HMD3	2.01	0.42
2:B4:435:HIS:O	2:B4:439:LEU:HG	2.19	0.42
2:B4:600:TRP:CE2	2:B4:604:HIS:CE1	3.08	0.42
2:B5:193:LEU:HD12	2:B5:273:ALA:HA	2.02	0.42
2:B6:181:LEU:HD11	14:B6:813:CLA:C4	2.43	0.42
2:B6:535:THR:HG21	2:B6:588:TRP:CZ2	2.53	0.42
2:B6:663:TRP:CE3	14:B6:804:CLA:HMA1	2.54	0.42
14:B6:810:CLA:H11	10:L5:148:ILE:CD1	2.50	0.42
3:C2:13:CYS:SG	3:C2:15:GLN:HB2	2.60	0.42
6:F4:88:VAL:HG11	6:F4:97:LYS:CB	2.46	0.42
7:I3:20:TRP:CD2	16:I3:102:BCR:HC31	2.55	0.42
8:J4:27:ILE:HG21	16:J4:104:BCR:C9	2.49	0.42
14:B1:854:CLA:H162	10:L2:56:TYR:CZ	2.54	0.42
14:B2:809:CLA:H13	10:L3:138:LEU:HD11	2.01	0.42
16:M4:101:BCR:H321	16:M4:101:BCR:HC8	2.00	0.42
13:P4:62:GLN:HB2	13:P4:76:LEU:HD12	2.01	0.42
1:A1:360:LEU:CD1	14:A1:829:CLA:HBB1	2.49	0.42
1:A1:681:PHE:CD1	16:A1:847:BCR:H363	2.54	0.42
14:A1:804:CLA:HMC3	14:A1:829:CLA:HMA1	2.01	0.42
16:A1:847:BCR:H20C	16:A1:847:BCR:H361	1.88	0.42
1:A3:90:MET:HE2	1:A3:143:LEU:HD11	2.01	0.42
1:A3:100:TYR:OH	1:A3:152:ILE:O	2.23	0.42
1:A3:431:ASP:O	1:A3:435:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:449:ILE:HD11	16:A3:856:BCR:C40	2.50	0.42
14:A3:806:CLA:H62	14:A3:806:CLA:H41	1.81	0.42
1:A4:545:THR:HA	1:A4:601:TRP:HZ3	1.84	0.42
14:A4:822:CLA:HBA2	14:A4:822:CLA:H3A	1.86	0.42
14:A4:838:CLA:HMB2	14:B4:834:CLA:H52	2.01	0.42
1:A5:114:ALA:O	1:A5:115:GLN:O	2.38	0.42
1:A5:257:ASP:O	1:A5:258:TRP:HB2	2.20	0.42
1:A5:404:LEU:HD21	14:A5:806:CLA:H142	2.02	0.42
1:A5:513:PHE:HE1	14:A5:827:CLA:HMC3	1.84	0.42
14:A5:841:CLA:O1A	14:A5:841:CLA:H2	2.19	0.42
1:A6:355:GLN:HG3	14:A6:1625:CLA:H152	2.01	0.42
1:A6:650:LEU:HD22	2:B6:657:LEU:CD2	2.49	0.42
2:B1:660:HIS:NE2	14:B1:804:CLA:CHB	2.82	0.42
14:B1:825:CLA:H41	14:B1:825:CLA:H61	1.77	0.42
2:B1:343:CYS:HA	14:B1:827:CLA:H51	2.01	0.42
2:B2:564:PRO:O	2:B2:565:CYS:CB	2.68	0.42
14:A2:1634:CLA:HMA1	2:B2:691:THR:OG1	2.19	0.42
2:B3:189:TRP:N	14:B3:1816:CLA:CBB	2.82	0.42
2:B3:313:LYS:O	2:B3:314:VAL:HG13	2.20	0.42
2:B3:353:GLN:HG3	14:B3:1827:CLA:O1D	2.20	0.42
2:B6:329:TYR:CE2	2:B6:336:GLN:HG2	2.55	0.42
2:B6:627:ARG:NH2	2:B6:628:ASP:OD2	2.39	0.42
14:B6:805:CLA:H122	16:I6:102:BCR:H281	2.01	0.42
5:E6:33:LYS:C	5:E6:35:PRO:HD3	2.40	0.42
8:J4:11:ALA:N	8:J4:12:PRO:HD2	2.34	0.42
14:A3:834:CLA:CGA	10:L3:62:TRP:CD1	3.03	0.42
10:L5:124:PHE:CZ	16:L5:207:BCR:H292	2.55	0.42
12:X2:30:TYR:CD2	12:X2:30:TYR:C	2.93	0.42
1:A1:468:PHE:CE2	14:B1:811:CLA:C1C	3.02	0.42
1:A1:212:TRP:HA	14:A1:813:CLA:HBB1	2.02	0.42
1:A2:443:HIS:CD2	14:A2:1633:CLA:HMB1	2.54	0.42
1:A2:508:THR:HG22	1:A2:510:SER:H	1.85	0.42
1:A3:366:LEU:HD11	14:A3:819:CLA:H52	2.02	0.42
1:A3:510:SER:HB3	1:A3:513:PHE:CE1	2.55	0.42
14:A3:819:CLA:O1A	14:A3:829:CLA:HMD1	2.20	0.42
1:A4:596:PHE:CE1	1:A4:600:PHE:HE1	2.38	0.42
1:A5:387:TYR:N	1:A5:388:PRO:CD	2.82	0.42
1:A5:466:ARG:O	2:B5:646:THR:CG2	2.67	0.42
1:A5:679:ALA:HB1	1:A5:738:GLY:O	2.20	0.42
14:A5:843:CLA:HBA1	14:A5:843:CLA:H3A	1.80	0.42
1:A5:744:TRP:CZ3	16:A5:850:BCR:H313	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A6:1605:CLA:C7	16:A6:1645:BCR:H402	2.50	0.42
14:A6:1621:CLA:HMB1	14:A6:1621:CLA:HBB1	2.01	0.42
14:A6:1640:CLA:O1A	14:A6:1640:CLA:H2	2.20	0.42
2:B1:430:LEU:HB3	14:B1:833:CLA:CED	2.49	0.42
2:B1:493:PRO:HG3	14:B1:837:CLA:ND	2.34	0.42
1:A1:724:ILE:HG12	2:B1:574:CYS:SG	2.60	0.42
2:B4:222:ALA:N	2:B4:223:PRO:CD	2.83	0.42
2:B4:696:LEU:HD21	10:L4:37:TYR:CE2	2.55	0.42
2:B5:398:VAL:HG23	2:B5:547:ALA:HB1	2.02	0.42
2:B6:89:ALA:HA	2:B6:112:VAL:HG12	2.02	0.42
14:B6:806:CLA:HBA1	14:B6:806:CLA:H3A	1.83	0.42
2:B6:318:PHE:HB2	14:B6:823:CLA:HMA1	2.01	0.42
14:B6:829:CLA:H8	19:B6:848:LMG:H242	2.01	0.42
3:C1:50:CYS:O	3:C1:51:LYS:HB2	2.20	0.42
6:F2:99:ILE:O	8:J2:11:ALA:N	2.51	0.42
6:F4:70:PHE:HB2	16:F4:201:BCR:C32	2.49	0.42
6:F5:76:TRP:CZ2	14:F5:1301:CLA:O1A	2.73	0.42
7:I2:22:MET:CE	16:I2:101:BCR:H331	2.49	0.42
7:I5:37:GLU:O	7:I5:38:ALA:HB3	2.19	0.42
10:L2:138:LEU:HD13	14:L2:207:CLA:CED	2.50	0.42
7:I4:20:TRP:HE3	14:L6:208:CLA:H13	1.84	0.42
11:M5:17:LEU:HB3	11:M5:18:PRO:CD	2.49	0.42
1:A1:114:ALA:O	1:A1:115:GLN:O	2.38	0.42
1:A1:300:HIS:HB2	14:A1:817:CLA:CHB	2.50	0.42
14:A2:1601:CLA:HBA2	14:A2:1601:CLA:H3A	1.74	0.42
14:A2:1629:CLA:HBB1	14:A2:1636:CLA:HMA2	2.02	0.42
15:A2:1646:PQN:H191	15:A2:1646:PQN:H212	1.90	0.42
1:A2:649:TRP:O	1:A2:653:PHE:HB3	2.20	0.42
1:A2:750:ARG:O	1:A2:754:VAL:HG22	2.20	0.42
1:A3:115:GLN:HE22	14:A3:808:CLA:C4B	2.33	0.42
1:A3:168:MET:O	1:A3:172:MET:HB2	2.20	0.42
1:A3:646:ILE:HG13	14:A3:802:CLA:C1	2.50	0.42
1:A3:649:TRP:O	1:A3:653:PHE:HB3	2.20	0.42
1:A4:118:TRP:HB3	16:J4:104:BCR:HC21	2.01	0.42
1:A5:447:VAL:HG21	14:A5:838:CLA:C2C	2.50	0.42
1:A5:622:TRP:O	1:A5:633:HIS:HD2	2.02	0.42
14:A6:1633:CLA:H2A	10:L6:65:LEU:O	2.20	0.42
2:B1:427:TRP:CE2	14:B1:832:CLA:HBB1	2.54	0.42
2:B1:688:HIS:HE1	2:B1:697:VAL:O	2.03	0.42
2:B1:216:PRO:HD2	14:B1:816:CLA:C2D	2.50	0.42
2:B2:456:ILE:CG2	2:B2:458:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:181:LEU:HD21	14:B2:804:CLA:H93	2.02	0.42
2:B2:389:ALA:HB1	16:B2:846:BCR:H372	2.02	0.42
16:B2:847:BCR:H361	16:B2:847:BCR:H20C	1.92	0.42
14:B3:1832:CLA:HBA2	14:B3:1832:CLA:H3A	1.56	0.42
2:B3:529:ILE:CG2	14:B3:1839:CLA:HAB	2.48	0.42
2:B3:216:PRO:HD2	14:B3:1817:CLA:CAD	2.50	0.42
2:B4:189:TRP:CZ2	2:B4:193:LEU:HD21	2.54	0.42
14:B4:808:CLA:H91	19:B4:851:LMG:H401	2.02	0.42
14:B5:1808:CLA:H91	19:B5:1851:LMG:H401	2.02	0.42
14:B5:1821:CLA:CMD	14:B5:1823:CLA:HBB1	2.49	0.42
2:B6:466:ILE:HG22	2:B6:470:HIS:CE1	2.55	0.42
2:B6:433:GLY:N	2:B6:531:LEU:HD13	2.35	0.42
2:B6:595:TRP:CE2	14:B6:804:CLA:H152	2.54	0.42
14:B6:820:CLA:HBB1	16:B6:843:BCR:H14C	2.01	0.42
4:D1:31:TRP:NE1	4:D1:49:MET:SD	2.88	0.42
6:F3:109:CYS:O	6:F3:112:THR:HB	2.20	0.42
7:I3:31:PHE:O	7:I3:35:GLU:HG2	2.20	0.42
7:I4:29:LEU:HD21	14:L6:206:CLA:HBC3	2.01	0.42
16:I5:102:BCR:H331	16:I5:102:BCR:C8	2.50	0.42
2:B6:91:TRP:CZ2	7:I6:12:TRP:HA	2.54	0.42
16:L1:209:BCR:H20C	16:L1:209:BCR:H361	1.88	0.42
2:B6:690:ARG:HH22	10:L6:14:VAL:HG22	1.84	0.42
7:I4:16:PRO:HB2	14:L6:208:CLA:H142	2.02	0.42
1:A1:514:GLY:HA2	1:A1:528:PRO:HB3	2.01	0.42
1:A2:75:ALA:HB1	14:A2:1607:CLA:HBB1	2.02	0.42
1:A2:646:ILE:HG13	14:A2:1603:CLA:H12	2.02	0.42
1:A3:120:ILE:O	1:A3:122:GLY:N	2.53	0.42
1:A3:281:PHE:CD1	14:A3:818:CLA:HMB1	2.55	0.42
1:A3:588:GLN:HA	1:A3:593:ASP:OD2	2.20	0.42
14:A3:808:CLA:HBA2	14:A3:808:CLA:H3A	1.77	0.42
1:A4:548:VAL:HB	1:A4:601:TRP:CE3	2.55	0.42
14:A4:827:CLA:H41	14:A4:827:CLA:H62	1.81	0.42
14:A4:838:CLA:HBB1	14:A4:839:CLA:HMD1	2.01	0.42
1:A5:283:GLY:O	1:A5:507:ALA:HB3	2.20	0.42
1:A5:28:TRP:CD1	14:A5:811:CLA:HBA2	2.55	0.42
1:A5:84:PHE:CE1	14:A5:805:CLA:C9	3.01	0.42
14:A6:1640:CLA:H41	14:A6:1640:CLA:H62	1.83	0.42
1:A6:34:PHE:CD1	1:A6:61:HIS:CE1	3.08	0.42
2:B1:17:THR:OG1	2:B1:704:VAL:HG22	2.20	0.42
1:A1:601:TRP:CH2	14:B1:801:CLA:HBB1	2.52	0.42
2:B1:538:LEU:HD21	14:B1:802:CLA:O2D	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B1:818:CLA:HBA2	14:B1:818:CLA:H3A	1.46	0.42
2:B2:236:PRO:O	2:B2:250:GLY:HA3	2.19	0.42
14:B3:1803:CLA:H62	14:B3:1803:CLA:H102	1.84	0.42
2:B3:284:ILE:O	2:B3:288:HIS:ND1	2.46	0.42
2:B4:220:GLY:O	2:B4:221:LEU:HB2	2.20	0.42
2:B4:42:TYR:CZ	2:B4:333:LEU:HD21	2.55	0.42
2:B4:440:TYR:CZ	2:B4:524:LEU:HB3	2.55	0.42
2:B4:634:SER:O	2:B4:638:ILE:HB	2.20	0.42
2:B4:58:LEU:HD22	14:B4:809:CLA:C9	2.50	0.42
14:B4:818:CLA:HBA2	14:B4:818:CLA:H3A	1.76	0.42
2:B5:222:ALA:HB3	2:B5:223:PRO:HD3	2.01	0.42
2:B6:14:ASP:OD2	2:B6:18:ARG:HB3	2.19	0.42
2:B6:339:TRP:HZ2	14:B6:824:CLA:CAB	2.32	0.42
6:F3:53:VAL:HG12	6:F3:63:PHE:HB2	2.02	0.42
7:I4:20:TRP:CE2	16:I4:102:BCR:HC32	2.53	0.42
8:J6:19:MET:CE	8:J6:19:MET:HA	2.50	0.42
16:L1:209:BCR:H392	10:L3:83:ILE:CD1	2.50	0.42
16:L6:201:BCR:H361	16:L6:201:BCR:H20C	1.89	0.42
10:L6:142:PHE:CD1	14:L6:208:CLA:H43	2.55	0.42
10:L6:96:TYR:C	10:L6:96:TYR:CD2	2.94	0.42
1:A1:24:SER:O	14:A1:810:CLA:HMA1	2.20	0.41
1:A1:613:PHE:O	1:A1:617:MET:HG2	2.19	0.41
14:A2:1621:CLA:CAD	14:A2:1631:CLA:H41	2.50	0.41
1:A2:292:LEU:HG	1:A2:378:PRO:O	2.20	0.41
1:A2:372:GLN:HA	1:A2:372:GLN:HE21	1.85	0.41
1:A2:702:GLU:CD	2:B2:551:LYS:HB2	2.40	0.41
14:A3:819:CLA:H3A	14:A3:819:CLA:HBA2	1.93	0.41
16:A3:852:BCR:H20C	16:A3:852:BCR:H361	1.87	0.41
16:A3:852:BCR:H402	14:B3:1802:CLA:C14	2.49	0.41
1:A4:36:ARG:NH1	13:P4:67:ASP:C	2.73	0.41
1:A4:587:CYS:HB2	2:B4:673:TRP:HB3	2.01	0.41
14:A4:820:CLA:H143	14:A4:823:CLA:H91	2.02	0.41
16:A4:847:BCR:H403	16:A4:847:BCR:H23C	2.02	0.41
1:A5:332:HIS:HA	14:A5:843:CLA:HBC2	2.02	0.41
1:A5:79:HIS:ND1	14:A5:805:CLA:O1A	2.53	0.41
1:A6:278:PHE:CD1	1:A6:279:LEU:HG	2.55	0.41
1:A6:74:SER:HA	1:A6:77:PHE:HD1	1.84	0.41
2:B1:171:GLU:HB3	2:B1:290:TYR:HB3	2.02	0.41
2:B1:660:HIS:CE1	2:B1:726:THR:HG21	2.55	0.41
2:B3:525:VAL:HG12	14:B3:1803:CLA:C14	2.50	0.41
2:B3:637:LEU:HD22	2:B3:730:PHE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:463:ALA:HB2	14:B4:840:CLA:O2D	2.20	0.41
2:B4:283:PHE:CE1	14:B4:821:CLA:CBB	3.02	0.41
2:B5:267:LEU:HD13	14:B5:1819:CLA:H2A	2.01	0.41
2:B5:189:TRP:CZ3	2:B5:192:HIS:CD2	3.08	0.41
2:B5:236:PRO:O	2:B5:250:GLY:HA3	2.19	0.41
2:B5:551:LYS:NZ	6:F5:137:THR:OG1	2.53	0.41
2:B5:682:GLU:HG2	3:C5:80:TYR:HE2	1.86	0.41
3:C4:28:VAL:HG12	4:D4:109:ARG:HB3	2.02	0.41
4:D3:43:THR:O	4:D3:44:ALA:CB	2.68	0.41
4:D4:95:HIS:HA	4:D4:97:LYS:N	2.35	0.41
6:F5:88:VAL:HG12	6:F5:94:ALA:HA	2.02	0.41
6:F4:65:ILE:HD12	14:J4:102:CLA:HMB3	1.98	0.41
10:L2:138:LEU:HD13	14:L2:207:CLA:HED2	2.01	0.41
10:L2:6:LYS:HB2	10:L2:7:PRO:HD2	2.02	0.41
10:L3:68:LEU:HD23	10:L3:68:LEU:N	2.35	0.41
14:L6:203:CLA:H191	14:L6:207:CLA:CBB	2.50	0.41
14:L6:208:CLA:H3A	14:L6:208:CLA:HBA1	1.88	0.41
16:M1:1202:BCR:H321	16:M1:1202:BCR:HC8	2.02	0.41
1:A1:16:VAL:HG11	1:A1:183:ARG:HB3	2.03	0.41
1:A1:377:MET:N	1:A1:378:PRO:CD	2.82	0.41
1:A1:679:ALA:HB1	1:A1:738:GLY:O	2.19	0.41
1:A1:744:TRP:CG	16:A1:847:BCR:HC22	2.56	0.41
1:A2:120:ILE:O	1:A2:122:GLY:N	2.53	0.41
14:A2:1610:CLA:H3A	14:A2:1610:CLA:HBA2	1.77	0.41
1:A2:178:PHE:CE2	14:A2:1612:CLA:C2D	3.03	0.41
1:A2:196:MET:HE1	14:A2:1627:CLA:H142	2.02	0.41
1:A2:221:LEU:CB	1:A2:222:PRO:HD3	2.50	0.41
1:A2:555:LYS:HD2	2:B2:680:LEU:HD13	2.02	0.41
1:A3:577:PRO:O	1:A3:578:CYS:CB	2.67	0.41
14:A3:805:CLA:C7	16:A3:849:BCR:H402	2.50	0.41
1:A4:19:ASP:N	1:A4:20:PRO:HD3	2.35	0.41
1:A5:302:LEU:HD13	14:A5:815:CLA:CMC	2.48	0.41
2:B3:372:ALA:HA	2:B3:600:TRP:CZ3	2.55	0.41
1:A4:581:PRO:HB3	2:B4:564:PRO:HB2	2.01	0.41
2:B5:153:TRP:HH2	14:B5:1801:CLA:C6	2.33	0.41
14:L4:205:CLA:H101	14:B5:1812:CLA:C9	2.50	0.41
2:B5:231:VAL:HA	2:B5:234:GLN:HG2	2.02	0.41
2:B5:514:LEU:HD12	14:B5:1828:CLA:HMC1	2.01	0.41
2:B6:220:GLY:O	2:B6:221:LEU:CB	2.68	0.41
2:B6:318:PHE:H	14:B6:822:CLA:C3B	2.33	0.41
2:B6:300:ILE:HG23	14:B6:819:CLA:CED	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:572:LEU:HD21	3:C1:52:ARG:NH2	2.35	0.41
7:I2:9:PHE:CZ	7:I2:10:LEU:CD1	3.03	0.41
8:J4:40:PRO:O	8:J4:41:LEU:HB2	2.20	0.41
10:L1:134:VAL:HG11	16:L1:209:BCR:C21	2.50	0.41
1:A1:473:ASP:OD1	10:L1:69:ARG:NH2	2.53	0.41
14:L4:203:CLA:H3A	14:L4:203:CLA:HBA2	1.87	0.41
13:P2:62:GLN:HB2	13:P2:76:LEU:HD12	2.01	0.41
1:A1:88:SER:HB2	1:A1:162:ALA:O	2.20	0.41
1:A1:237:PRO:CB	1:A1:248:LEU:HD21	2.51	0.41
1:A1:379:PRO:HB2	14:A1:818:CLA:HAA2	2.02	0.41
14:A1:839:CLA:HBB1	14:A1:839:CLA:HHC	2.01	0.41
1:A2:90:MET:CE	14:A2:1610:CLA:HED2	2.46	0.41
1:A2:682:ILE:HD11	16:A2:1652:BCR:C14	2.51	0.41
1:A3:45:THR:HG21	14:A3:841:CLA:C4B	2.51	0.41
1:A3:657:GLN:HG2	1:A3:750:ARG:NH2	2.35	0.41
14:A3:843:CLA:H62	14:A3:843:CLA:H41	1.68	0.41
1:A5:699:GLU:O	1:A5:702:GLU:HB2	2.20	0.41
1:A5:116:VAL:O	14:A5:809:CLA:HED2	2.20	0.41
1:A5:212:TRP:N	14:A5:814:CLA:HBB1	2.36	0.41
14:A5:834:CLA:HMD2	14:A5:835:CLA:HBB1	2.01	0.41
1:A5:447:VAL:HG21	14:A5:838:CLA:HMC3	2.01	0.41
1:A6:196:MET:SD	14:A6:1625:CLA:HMD1	2.60	0.41
1:A6:744:TRP:CG	16:A6:1648:BCR:HC22	2.55	0.41
2:B1:56:ILE:O	2:B1:60:VAL:HG23	2.20	0.41
2:B1:447:VAL:HG11	2:B1:621:TYR:CZ	2.55	0.41
14:B1:806:CLA:H122	16:I1:102:BCR:H281	2.02	0.41
2:B1:50:PHE:CZ	14:B1:814:CLA:HED1	2.55	0.41
2:B1:342:ALA:HB1	16:B1:847:BCR:C20	2.50	0.41
2:B2:264:THR:HG22	2:B2:363:PHE:CE1	2.54	0.41
2:B2:432:LEU:HD11	14:B2:837:CLA:CMB	2.51	0.41
2:B2:500:LEU:N	2:B2:501:PRO:CD	2.83	0.41
14:B2:805:CLA:H41	14:B2:805:CLA:H61	1.70	0.41
2:B3:233:ALA:HB2	14:B3:1818:CLA:HMA2	2.02	0.41
2:B3:625:TRP:CZ2	14:B3:1803:CLA:H142	2.55	0.41
2:B4:25:ALA:HB2	19:B4:851:LMG:C12	2.38	0.41
2:B4:481:LEU:HD11	14:B4:836:CLA:OBD	2.20	0.41
2:B4:504:LEU:HA	2:B4:507:ILE:HG22	2.03	0.41
1:A4:121:VAL:HB	14:B4:835:CLA:HMD1	2.01	0.41
2:B5:60:VAL:HG21	14:B5:1830:CLA:H11	2.01	0.41
2:B5:466:ILE:HD13	14:B5:1836:CLA:HBB1	2.02	0.41
2:B5:380:TYR:CD1	2:B5:593:ILE:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B5:456:ILE:HD11	14:B5:1835:CLA:CHB	2.50	0.41
2:B5:497:ASN:HB3	2:B5:500:LEU:HB2	2.01	0.41
2:B6:157:GLN:O	2:B6:161:ARG:HG3	2.20	0.41
2:B6:26:MET:CE	19:B6:848:LMG:HC3	2.50	0.41
2:B6:493:PRO:HG3	14:B6:836:CLA:C2D	2.49	0.41
2:B6:339:TRP:NE1	14:B6:824:CLA:C2B	2.70	0.41
5:E6:57:THR:HG23	13:P6:42:ALA:CB	2.50	0.41
7:I2:28:GLY:O	7:I2:32:LEU:HG	2.20	0.41
14:B3:1805:CLA:H122	16:I3:101:BCR:H281	2.02	0.41
7:I3:30:LEU:HD13	16:L3:206:BCR:C8	2.50	0.41
7:I6:25:VAL:HG12	7:I6:29:LEU:HD12	2.02	0.41
16:B1:852:BCR:C21	8:J1:36:LEU:HD22	2.50	0.41
10:L1:153:PHE:O	10:L1:154:ASN:HB2	2.21	0.41
10:L1:68:LEU:HD13	10:L1:73:VAL:HG23	2.01	0.41
10:L2:23:ASP:O	10:L2:23:ASP:CG	2.58	0.41
2:B6:142:LEU:HD23	11:M6:14:ILE:HG22	2.02	0.41
1:A4:36:ARG:NH1	13:P4:67:ASP:CA	2.83	0.41
1:A1:401:GLY:O	1:A1:405:VAL:HG23	2.21	0.41
1:A2:280:THR:OG1	1:A2:296:ASP:OD1	2.23	0.41
1:A2:40:ARG:HD3	13:P2:61:ASP:C	2.40	0.41
1:A2:626:ALA:HB1	1:A2:627:PRO:HD2	2.02	0.41
1:A2:466:ARG:NH2	1:A2:641:GLN:O	2.53	0.41
1:A3:446:TRP:CE2	14:A3:832:CLA:HAB	2.55	0.41
1:A3:56:HIS:HB3	14:A3:805:CLA:HAB	2.02	0.41
14:A3:821:CLA:H143	14:A3:824:CLA:H91	2.02	0.41
1:A3:592:TRP:CD1	14:A3:830:CLA:HMD1	2.56	0.41
1:A4:323:HIS:HB3	1:A4:328:ILE:HD11	2.01	0.41
1:A4:586:THR:O	1:A4:589:VAL:HG13	2.20	0.41
1:A5:377:MET:N	1:A5:378:PRO:CD	2.83	0.41
1:A5:542:HIS:HE1	1:A5:612:HIS:ND1	2.18	0.41
1:A6:404:LEU:HD21	14:A6:1606:CLA:H142	2.01	0.41
14:A6:1608:CLA:HBA2	14:A6:1608:CLA:H3A	1.76	0.41
1:A6:592:TRP:CD1	14:A6:1630:CLA:HMD1	2.55	0.41
1:A6:203:GLY:O	1:A6:207:LEU:HB2	2.20	0.41
1:A6:456:PHE:HB2	1:A6:541:ILE:HD11	2.02	0.41
14:B1:801:CLA:O1A	14:B1:801:CLA:H3A	2.20	0.41
2:B1:177:HIS:HB2	14:B1:825:CLA:HED3	2.01	0.41
2:B2:391:ALA:O	2:B2:395:ILE:HG13	2.20	0.41
14:B3:1826:CLA:H41	14:B3:1826:CLA:H61	1.77	0.41
2:B3:231:VAL:HA	2:B3:234:GLN:HG2	2.02	0.41
2:B4:339:TRP:CH2	16:B4:848:BCR:H372	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:376:THR:HG23	2:B4:597:THR:CG2	2.51	0.41
2:B4:711:ALA:HB2	15:B4:844:PQN:C7	2.50	0.41
1:A5:684:ALA:HB2	14:B5:1804:CLA:C3D	2.50	0.41
2:B6:288:HIS:C	14:B6:821:CLA:HAC2	2.40	0.41
14:B6:841:CLA:H3A	14:B6:841:CLA:HBA2	1.88	0.41
3:C5:17:VAL:HG11	4:D5:102:PRO:HB2	2.02	0.41
4:D3:95:HIS:HA	4:D3:97:LYS:N	2.35	0.41
4:D4:43:THR:O	4:D4:44:ALA:CB	2.68	0.41
4:D6:117:ARG:HG3	4:D6:121:GLN:HB2	2.03	0.41
4:D6:83:TYR:CD1	4:D6:83:TYR:N	2.88	0.41
2:B1:548:ARG:HD3	6:F1:141:ARG:O	2.20	0.41
16:J5:103:BCR:H11C	16:J5:103:BCR:H341	1.94	0.41
10:L6:48:LEU:HD22	10:L6:52:MET:SD	2.60	0.41
11:M2:26:SER:HA	11:M2:29:LEU:HD12	2.01	0.41
14:B4:806:CLA:C2	11:M4:26:SER:HB2	2.51	0.41
1:A2:36:ARG:NH1	13:P2:67:ASP:CA	2.84	0.41
13:P6:46:SER:HB3	13:P6:64:PHE:CE1	2.56	0.41
12:X2:23:ASN:OD1	14:X2:1701:CLA:NA	2.53	0.41
14:A1:809:CLA:HBA2	14:A1:809:CLA:H3A	1.71	0.41
1:A1:281:PHE:HE1	14:A1:817:CLA:HAB	1.84	0.41
1:A1:304:ILE:HD12	14:A1:818:CLA:HAB	2.03	0.41
14:A2:1637:CLA:H3A	14:A2:1637:CLA:HBA2	1.78	0.41
1:A2:283:GLY:O	1:A2:507:ALA:HB3	2.19	0.41
1:A3:180:TYR:OH	14:A3:811:CLA:CGD	2.68	0.41
1:A3:436:HIS:CD2	1:A3:440:ILE:HG13	2.55	0.41
14:A3:805:CLA:HMC3	14:A3:830:CLA:HMA1	2.02	0.41
14:A3:809:CLA:CBB	14:B3:1835:CLA:HMD2	2.50	0.41
14:A3:845:CLA:H3A	14:A3:845:CLA:HBA1	1.79	0.41
1:A4:697:TRP:CZ2	15:A4:843:PQN:H2M3	2.55	0.41
1:A5:120:ILE:O	1:A5:122:GLY:N	2.53	0.41
1:A5:696:TYR:CD2	1:A5:696:TYR:C	2.93	0.41
1:A5:396:HIS:HB2	14:A5:828:CLA:CHB	2.51	0.41
14:A6:1621:CLA:H143	14:A6:1624:CLA:H91	2.03	0.41
1:A6:168:MET:O	1:A6:172:MET:HB2	2.20	0.41
2:B1:349:SER:O	2:B1:353:GLN:HG2	2.21	0.41
2:B1:456:ILE:HD11	14:B1:834:CLA:C4A	2.49	0.41
2:B1:637:LEU:HD22	2:B1:730:PHE:HA	2.01	0.41
2:B1:657:LEU:HB3	14:B1:801:CLA:O2A	2.20	0.41
14:B1:803:CLA:HMB2	14:B1:833:CLA:H52	2.01	0.41
14:B1:826:CLA:HBB1	14:B1:840:CLA:HBB	2.03	0.41
2:B2:25:ALA:HB1	19:B2:848:LMG:O8	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:52:HIS:CD2	14:B2:804:CLA:HMA1	2.55	0.41
2:B2:150:PHE:CE2	14:B2:810:CLA:HBC3	2.55	0.41
2:B3:318:PHE:CE1	16:B3:1848:BCR:H353	2.55	0.41
2:B3:236:PRO:O	2:B3:250:GLY:HA3	2.19	0.41
14:B4:832:CLA:HBC2	16:B4:848:BCR:H402	2.02	0.41
14:B4:852:CLA:HBA2	14:B4:852:CLA:H12	1.88	0.41
2:B5:442:HIS:HB2	14:B5:1835:CLA:CHC	2.50	0.41
2:B5:229:TRP:CB	14:B5:1818:CLA:HBA2	2.51	0.41
2:B5:52:HIS:CE1	14:B5:1807:CLA:HMA2	2.56	0.41
2:B5:629:TYR:O	2:B5:633:ASN:HB2	2.19	0.41
2:B6:166:TRP:CZ2	14:B6:813:CLA:CAC	3.03	0.41
2:B6:182:PHE:N	2:B6:182:PHE:HD2	2.18	0.41
2:B6:263:GLN:HB3	2:B6:263:GLN:HE21	1.59	0.41
2:B6:84:ARG:HA	2:B6:84:ARG:CZ	2.51	0.41
14:J1:101:CLA:HBA2	14:J1:101:CLA:H3A	1.70	0.41
10:L4:134:VAL:O	10:L4:138:LEU:HG	2.21	0.41
10:L5:54:HIS:HA	10:L5:57:PHE:CE2	2.56	0.41
1:A1:537:MET:SD	1:A1:644:ILE:HG22	2.61	0.41
16:A2:1650:BCR:H403	16:A2:1650:BCR:H23C	2.03	0.41
1:A2:387:TYR:OH	1:A2:524:VAL:O	2.25	0.41
1:A2:718:GLN:HA	1:A2:719:PRO:HD3	1.87	0.41
1:A3:177:TRP:HD1	14:A3:811:CLA:CHC	2.34	0.41
1:A4:156:PHE:CE2	14:A4:815:CLA:HED2	2.56	0.41
1:A4:649:TRP:O	1:A4:653:PHE:HB3	2.21	0.41
14:A4:807:CLA:H3A	14:A4:807:CLA:HBA2	1.76	0.41
14:A4:826:CLA:HBB1	14:A4:833:CLA:HMA2	2.03	0.41
1:A4:575:ARG:NH2	17:A4:850:LHG:O2	2.52	0.41
1:A5:360:LEU:HD23	1:A5:407:GLY:C	2.41	0.41
14:A5:809:CLA:CBB	14:B5:1835:CLA:HMD2	2.50	0.41
1:A5:90:MET:HE3	14:A5:808:CLA:HED2	2.02	0.41
16:A6:1646:BCR:H403	16:A6:1646:BCR:H23C	2.02	0.41
1:A6:67:ASP:O	1:A6:71:LYS:HG3	2.21	0.41
2:B1:275:HIS:HB2	14:B1:818:CLA:C4A	2.50	0.41
2:B2:50:PHE:HB3	2:B2:148:ALA:O	2.21	0.41
2:B2:636:GLN:HG3	2:B2:737:ALA:HB1	2.01	0.41
2:B3:320:MET:HA	2:B3:321:PRO:HD3	1.95	0.41
2:B3:390:PHE:CB	2:B3:540:LEU:HD22	2.51	0.41
1:A4:332:HIS:HA	14:B5:1801:CLA:HBC2	2.03	0.41
2:B5:676:TYR:C	2:B5:676:TYR:CD2	2.93	0.41
2:B6:234:GLN:O	2:B6:236:PRO:HD3	2.20	0.41
2:B6:361:TYR:O	2:B6:364:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B6:181:LEU:HD21	14:B6:806:CLA:H93	2.02	0.41
2:B6:466:ILE:HD11	14:B6:837:CLA:H43	2.02	0.41
1:A2:561:ARG:NE	4:D2:40:GLU:OE2	2.49	0.41
4:D6:134:LYS:HG2	4:D6:136:TYR:OH	2.21	0.41
4:D6:96:PRO:O	4:D6:97:LYS:C	2.59	0.41
7:I5:22:MET:O	7:I5:23:PRO:C	2.55	0.41
10:L3:57:PHE:C	10:L3:57:PHE:CD1	2.94	0.41
10:L4:50:VAL:HA	14:L4:204:CLA:O1D	2.20	0.41
10:L4:97:GLY:CA	10:L4:117:TRP:HD1	2.34	0.41
10:L6:153:PHE:O	10:L6:154:ASN:HB2	2.21	0.41
14:B4:812:CLA:H101	14:L6:208:CLA:C9	2.51	0.41
16:M3:1602:BCR:HC8	16:M3:1602:BCR:H321	2.03	0.41
5:E2:37:ILE:HD13	13:P2:41:ARG:CD	2.50	0.41
5:E4:37:ILE:HG21	13:P4:41:ARG:HD3	2.01	0.41
13:P4:54:GLU:HG2	13:P4:87:LYS:HB3	2.02	0.41
1:A1:577:PRO:O	1:A1:578:CYS:CB	2.67	0.41
14:A1:825:CLA:H3A	14:A1:825:CLA:HBA2	1.90	0.41
14:A2:1614:CLA:HHC	14:A2:1614:CLA:HBB1	2.02	0.41
14:A2:1625:CLA:HBA2	14:A2:1625:CLA:H3A	1.86	0.41
1:A2:88:SER:HB2	1:A2:162:ALA:O	2.20	0.41
1:A2:220:SER:O	1:A2:224:ASN:HB2	2.20	0.41
1:A4:406:VAL:HG11	1:A4:599:LEU:HG	2.03	0.41
1:A5:253:TYR:HA	1:A5:277:ASP:CG	2.41	0.41
1:A6:212:TRP:N	14:A6:1614:CLA:HBB1	2.36	0.41
14:A6:1605:CLA:HMC3	14:A6:1630:CLA:HMA1	2.02	0.41
1:A6:33:HIS:CG	1:A6:34:PHE:N	2.88	0.41
2:B1:629:TYR:O	2:B1:633:ASN:HB2	2.21	0.41
2:B1:267:LEU:HD13	14:B1:818:CLA:H2A	2.01	0.41
2:B1:354:HIS:CE1	14:B1:827:CLA:C1B	3.04	0.41
1:A2:585:GLY:HA3	2:B2:674:ARG:HD3	2.02	0.41
2:B3:531:LEU:HD21	14:B3:1804:CLA:CBB	2.51	0.41
2:B4:217:HIS:CG	2:B4:218:PRO:HD2	2.56	0.41
2:B4:342:ALA:HB2	16:B4:849:BCR:H372	2.02	0.41
2:B5:189:TRP:CH2	2:B5:192:HIS:CD2	3.08	0.41
2:B5:231:VAL:O	2:B5:234:GLN:HG2	2.21	0.41
2:B6:182:PHE:CD2	2:B6:182:PHE:N	2.87	0.41
2:B6:641:TYR:HB2	2:B6:646:THR:HG22	2.02	0.41
3:C2:11:ILE:HD12	13:P2:39:SER:O	2.21	0.41
4:D3:39:PHE:CE2	4:D3:47:ALA:HB3	2.56	0.41
10:L4:69:ARG:NH2	14:L4:201:CLA:HED3	2.36	0.41
1:A5:460:VAL:HG23	14:L5:203:CLA:HMC3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M4:17:LEU:HB3	11:M4:18:PRO:CD	2.51	0.41
1:A2:40:ARG:CG	13:P2:60:SER:CB	2.98	0.41
13:P3:46:SER:HB3	13:P3:64:PHE:CE1	2.56	0.41
13:P5:46:SER:HB3	13:P5:64:PHE:CE1	2.55	0.41
13:P6:54:GLU:HG2	13:P6:87:LYS:HB3	2.02	0.41
1:A2:114:ALA:O	1:A2:115:GLN:O	2.39	0.41
14:A2:1643:CLA:H41	14:A2:1643:CLA:H62	1.83	0.41
1:A2:177:TRP:HB2	14:A2:1613:CLA:CMC	2.51	0.41
1:A3:446:TRP:CD1	14:A3:843:CLA:O1A	2.74	0.41
1:A4:168:MET:O	1:A4:172:MET:HB2	2.21	0.41
1:A4:548:VAL:HG11	1:A4:601:TRP:CZ2	2.56	0.41
14:A4:811:CLA:HHC	14:A4:811:CLA:HBB1	2.02	0.41
1:A5:232:ALA:O	1:A5:235:ASP:HB2	2.20	0.41
1:A5:98:SER:HB2	1:A5:113:SER:O	2.20	0.41
1:A6:742:THR:HG21	14:A6:1602:CLA:CHA	2.51	0.41
2:B1:220:GLY:O	2:B1:221:LEU:CB	2.68	0.41
2:B1:380:TYR:CE1	2:B1:593:ILE:HG22	2.55	0.41
1:A1:662:ILE:O	2:B1:627:ARG:HD3	2.20	0.41
2:B1:595:TRP:CD1	14:B1:804:CLA:H152	2.55	0.41
2:B1:667:PHE:CB	14:B1:806:CLA:HMC3	2.50	0.41
2:B1:136:GLN:HE22	14:B1:815:CLA:HBD	1.86	0.41
2:B2:117:SER:HA	14:B2:826:CLA:HMA2	2.02	0.41
2:B2:339:TRP:CZ3	16:B2:845:BCR:H372	2.56	0.41
2:B2:593:ILE:HD13	2:B2:593:ILE:N	2.35	0.41
1:A2:597:LEU:HD21	2:B2:672:SER:CB	2.51	0.41
2:B2:298:HIS:CE1	14:B2:821:CLA:OBD	2.73	0.41
2:B3:496:GLY:O	2:B3:497:ASN:C	2.59	0.41
2:B4:623:MET:SD	2:B4:626:LEU:HD23	2.60	0.41
2:B4:211:PHE:HB3	14:B4:816:CLA:CMD	2.51	0.41
14:B4:836:CLA:HBA2	14:B4:837:CLA:HMB3	2.03	0.41
2:B4:153:TRP:CZ3	14:B4:852:CLA:H62	2.54	0.41
2:B5:235:ASN:OD1	2:B5:235:ASN:N	2.51	0.41
2:B5:263:GLN:HB3	2:B5:263:GLN:HE21	1.71	0.41
2:B5:30:PHE:CD1	2:B5:45:ILE:HD13	2.55	0.41
2:B6:496:GLY:O	2:B6:497:ASN:C	2.59	0.41
5:E1:7:VAL:O	5:E1:20:VAL:HA	2.20	0.41
5:E2:57:THR:HG21	13:P2:42:ALA:CA	2.50	0.41
5:E5:39:ARG:NH2	13:P5:24:TYR:HH	2.11	0.41
16:I4:102:BCR:H331	16:I4:102:BCR:C8	2.51	0.41
8:J2:27:ILE:HG21	16:J2:103:BCR:H343	2.02	0.41
16:L1:203:BCR:H331	16:L1:203:BCR:C8	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L2:44:ILE:HG23	10:L2:45:LEU:N	2.36	0.41
14:L4:203:CLA:H171	7:I5:24:THR:CG2	2.51	0.41
10:L5:25:GLY:O	10:L5:26:LEU:C	2.58	0.41
10:L5:58:LEU:HD23	10:L5:58:LEU:HA	1.89	0.41
11:M1:15:ALA:O	11:M1:18:PRO:HD2	2.21	0.41
13:P1:46:SER:HB3	13:P1:64:PHE:CE1	2.56	0.41
1:A1:436:HIS:CD2	1:A1:440:ILE:HG13	2.55	0.41
1:A2:744:TRP:CZ2	14:A2:1630:CLA:H11	2.56	0.41
1:A2:307:LEU:HD23	1:A2:307:LEU:HA	1.97	0.41
1:A3:257:ASP:O	1:A3:258:TRP:HB2	2.21	0.41
1:A4:114:ALA:O	1:A4:115:GLN:O	2.38	0.41
14:A4:833:CLA:HMD2	14:A4:834:CLA:HBB1	2.03	0.41
1:A5:466:ARG:O	2:B5:646:THR:HG21	2.21	0.41
1:A6:212:TRP:HA	14:A6:1614:CLA:HBB1	2.03	0.41
1:A6:88:SER:HB2	1:A6:162:ALA:O	2.21	0.41
2:B1:261:HIS:HA	2:B1:268:TRP:CZ2	2.56	0.41
2:B1:313:LYS:O	2:B1:314:VAL:HG13	2.20	0.41
2:B1:418:LYS:HG3	2:B1:419:GLU:N	2.35	0.41
2:B1:430:LEU:HD21	14:B1:803:CLA:CMD	2.51	0.41
14:B1:810:CLA:O1A	14:B1:828:CLA:HBD	2.21	0.41
2:B2:286:ALA:HB2	14:B2:818:CLA:HBC2	2.03	0.41
14:B3:1842:CLA:HED3	7:I3:31:PHE:CZ	2.54	0.41
2:B3:527:HIS:CD2	16:B3:1851:BCR:H322	2.55	0.41
2:B4:235:ASN:HA	2:B4:236:PRO:HD3	1.95	0.41
2:B5:440:TYR:CD1	14:B5:1803:CLA:H203	2.56	0.41
2:B5:503:TRP:HE3	14:B5:1819:CLA:H11	1.86	0.41
2:B5:582:PHE:CZ	14:B5:1831:CLA:HMD2	2.56	0.41
2:B6:390:PHE:CB	2:B6:540:LEU:HD22	2.50	0.41
2:B6:398:VAL:HG23	2:B6:547:ALA:HB1	2.02	0.41
2:B6:699:TRP:O	2:B6:699:TRP:CD1	2.74	0.41
14:B6:803:CLA:HMB2	14:B6:832:CLA:H52	2.02	0.41
4:D1:120:GLY:HA3	5:E1:13:GLU:OE2	2.21	0.41
7:I4:20:TRP:CD1	16:I4:102:BCR:HC22	2.48	0.41
8:J5:11:ALA:N	8:J5:12:PRO:HD2	2.35	0.41
8:J6:40:PRO:O	8:J6:41:LEU:HB2	2.21	0.41
10:L1:62:TRP:CE3	10:L1:81:SER:CB	3.04	0.41
10:L3:153:PHE:O	10:L3:154:ASN:HB2	2.21	0.41
14:A4:831:CLA:C3D	10:L4:21:ILE:HG21	2.51	0.41
13:P1:54:GLU:HG2	13:P1:87:LYS:HB3	2.01	0.41
1:A2:36:ARG:HH12	13:P2:71:GLU:HG3	1.79	0.41
1:A1:302:LEU:HD13	14:A1:814:CLA:HMC1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:337:THR:OG1	17:A2:1654:LHG:HC32	2.21	0.41
1:A2:519:ALA:HB2	1:A2:625:VAL:HG21	2.03	0.41
1:A3:281:PHE:CD1	14:A3:818:CLA:CMB	3.04	0.41
16:A3:852:BCR:H381	14:B3:1834:CLA:HMA1	2.03	0.41
14:A4:818:CLA:O1A	14:A4:828:CLA:HMD1	2.21	0.41
14:A6:1628:CLA:H41	14:A6:1628:CLA:H62	1.80	0.41
1:A6:682:ILE:HD12	16:A6:1648:BCR:H353	2.03	0.41
1:A6:681:PHE:CD1	16:A6:1648:BCR:H363	2.56	0.41
2:B1:189:TRP:CZ2	14:B1:819:CLA:OBD	2.74	0.41
2:B1:208:TRP:CH2	16:B1:845:BCR:H362	2.55	0.41
2:B1:595:TRP:CZ2	14:B1:805:CLA:C1B	3.04	0.41
2:B1:604:HIS:HB3	2:B1:608:TRP:CH2	2.56	0.41
2:B1:52:HIS:CG	14:B1:807:CLA:HMA1	2.56	0.41
14:B1:853:CLA:HMA2	14:A2:1601:CLA:HAA1	2.03	0.41
2:B2:551:LYS:HD3	6:F2:138:VAL:C	2.41	0.41
2:B2:278:ALA:HA	14:B2:815:CLA:HMC3	2.03	0.41
2:B2:339:TRP:NE1	14:B2:823:CLA:C2B	2.58	0.41
2:B3:340:HIS:CD2	14:B3:1807:CLA:H142	2.56	0.41
14:B3:1840:CLA:C1A	14:B3:1840:CLA:CGA	2.98	0.41
2:B3:254:LEU:HD22	2:B3:274:HIS:HA	2.02	0.41
2:B4:181:LEU:HD13	14:B4:815:CLA:CHB	2.49	0.41
2:B4:215:MET:HA	2:B4:216:PRO:HD3	1.90	0.41
2:B4:231:VAL:O	2:B4:234:GLN:HG2	2.21	0.41
2:B4:208:TRP:CZ2	14:B4:816:CLA:C2	3.04	0.41
2:B5:699:TRP:CD1	2:B5:702:LYS:HA	2.56	0.41
2:B6:178:LEU:O	2:B6:283:PHE:HB3	2.21	0.41
2:B6:354:HIS:CE1	14:B6:826:CLA:C1B	3.03	0.41
14:B6:818:CLA:HBA2	14:B6:818:CLA:H3A	1.96	0.41
3:C6:72:THR:H	3:C6:75:SER:HG	1.64	0.41
4:D6:29:ILE:HA	4:D6:81:LYS:O	2.21	0.41
6:F2:52:VAL:CG1	6:F2:54:ASP:HB2	2.50	0.41
6:F3:95:ASN:ND2	6:F3:95:ASN:H	2.19	0.41
7:I2:23:PRO:HA	7:I2:26:VAL:HG22	2.03	0.41
16:M2:1202:BCR:H321	16:M2:1202:BCR:HC8	2.01	0.41
11:M3:21:LEU:CD2	14:M3:1601:CLA:CMA	2.98	0.41
12:X1:30:TYR:CD2	12:X1:30:TYR:C	2.94	0.41
14:A1:804:CLA:C7	16:A1:844:BCR:H402	2.51	0.41
14:A2:1623:CLA:H143	14:A2:1626:CLA:H91	2.03	0.41
14:A2:1604:CLA:C14	16:A2:1652:BCR:H402	2.50	0.41
1:A2:257:ASP:O	1:A2:258:TRP:HB2	2.21	0.41
1:A2:452:GLY:CA	1:A2:544:PHE:CE1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:48:ILE:HD11	14:A2:1642:CLA:HMA1	2.02	0.41
1:A2:514:GLY:HA2	1:A2:528:PRO:HB3	2.03	0.41
1:A3:303:ALA:HB2	14:A3:818:CLA:CBB	2.46	0.41
1:A3:79:HIS:CE1	14:A3:805:CLA:CMA	3.04	0.41
1:A4:212:TRP:N	14:A4:813:CLA:HBB1	2.35	0.41
1:A6:612:HIS:ND1	14:A6:1636:CLA:HMC2	2.35	0.41
1:A6:750:ARG:O	1:A6:754:VAL:HG22	2.22	0.41
2:B1:50:PHE:CD1	2:B1:152:GLY:HA2	2.55	0.41
2:B1:660:HIS:HB3	14:B1:801:CLA:HBD	2.03	0.41
2:B1:668:MET:HA	14:B1:806:CLA:C3C	2.51	0.41
2:B1:711:ALA:HB2	15:B1:842:PQN:C7	2.50	0.41
2:B1:258:GLY:HA2	14:B1:818:CLA:H12	2.03	0.41
2:B1:493:PRO:CG	14:B1:837:CLA:C1D	2.86	0.41
14:B1:815:CLA:HMA2	16:B1:845:BCR:H282	2.03	0.41
2:B2:343:CYS:HA	14:B2:825:CLA:H51	2.02	0.41
2:B2:395:ILE:HG13	2:B2:561:TYR:CE1	2.56	0.41
2:B2:481:LEU:HA	2:B2:489:SER:OG	2.21	0.41
14:B3:1807:CLA:H3A	14:B3:1807:CLA:HBA1	1.83	0.41
14:B3:1811:CLA:H102	14:B3:1829:CLA:H193	2.02	0.41
2:B3:198:ILE:HB	2:B3:199:PRO:HD3	2.03	0.41
1:A4:724:ILE:CD1	2:B4:574:CYS:SG	3.09	0.41
14:B4:809:CLA:HBB1	14:B4:809:CLA:HHC	2.01	0.41
14:B5:1805:CLA:H122	16:I5:101:BCR:H281	2.03	0.41
2:B5:229:TRP:HB2	14:B5:1818:CLA:HBA2	2.02	0.41
2:B5:564:PRO:O	2:B5:565:CYS:HB3	2.20	0.41
2:B5:586:MET:O	2:B5:590:LEU:HG	2.21	0.41
2:B6:625:TRP:O	2:B6:629:TYR:HB3	2.21	0.41
3:C2:54:GLU:CG	3:C2:62:LEU:HD13	2.51	0.41
3:C2:65:ARG:HG2	3:C2:67:TYR:CZ	2.56	0.41
4:D6:43:THR:O	4:D6:44:ALA:CB	2.68	0.41
6:F4:70:PHE:CD1	16:F4:201:BCR:C9	3.04	0.41
8:J5:28:GLU:HG3	14:J5:101:CLA:NB	2.35	0.41
8:J6:27:ILE:HG21	16:J6:1105:BCR:C9	2.51	0.41
14:A6:1640:CLA:H192	8:J6:22:THR:CG2	2.51	0.41
14:K5:101:CLA:HBA2	14:K5:101:CLA:H3A	1.81	0.41
10:L2:65:LEU:O	14:L2:202:CLA:HED2	2.21	0.41
10:L5:7:PRO:HB3	10:L5:12:PRO:HA	2.03	0.41
10:L5:96:TYR:O	10:L5:100:SER:N	2.53	0.41
10:L6:36:ALA:HB3	10:L6:37:TYR:CD1	2.56	0.41
16:M5:101:BCR:HC8	16:M5:101:BCR:H321	2.02	0.41
16:M6:1202:BCR:H321	16:M6:1202:BCR:HC8	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:219:VAL:C	1:A1:222:PRO:HD2	2.41	0.40
1:A1:544:PHE:CZ	14:B1:801:CLA:HBB1	2.56	0.40
1:A1:622:TRP:O	1:A1:633:HIS:HD2	2.04	0.40
14:A2:1636:CLA:HMD2	14:A2:1637:CLA:HBB1	2.03	0.40
1:A2:429:VAL:O	1:A2:433:VAL:HG13	2.20	0.40
1:A3:114:ALA:O	1:A3:115:GLN:O	2.39	0.40
1:A3:16:VAL:HG11	1:A3:183:ARG:HB3	2.02	0.40
1:A3:375:TYR:OH	14:A3:837:CLA:HBC3	2.21	0.40
1:A3:543:ALA:HB1	14:A3:838:CLA:HMB3	2.03	0.40
1:A3:654:LEU:HD11	14:A3:801:CLA:H72	2.01	0.40
1:A3:75:ALA:HB1	14:A3:805:CLA:HBB1	2.01	0.40
1:A5:300:HIS:HB2	14:A5:818:CLA:C1B	2.51	0.40
14:A5:812:CLA:HHC	14:A5:812:CLA:HBB1	2.03	0.40
1:A6:198:ASN:OD1	1:A6:315:TYR:CD1	2.72	0.40
2:B1:178:LEU:HD21	14:B1:820:CLA:C1B	2.51	0.40
2:B2:217:HIS:CG	2:B2:218:PRO:HD2	2.56	0.40
2:B2:599:TYR:CE2	14:B2:836:CLA:C2C	3.04	0.40
2:B2:660:HIS:CE1	2:B2:726:THR:HG21	2.56	0.40
2:B3:110:ASN:HB2	2:B3:111:PRO:CD	2.51	0.40
14:B3:1820:CLA:H62	14:B3:1820:CLA:H41	1.76	0.40
2:B3:360:PRO:CB	14:B3:1820:CLA:HAA2	2.50	0.40
14:B3:1831:CLA:H8	19:B3:1850:LMG:H242	2.02	0.40
2:B3:599:TYR:CE2	14:B3:1839:CLA:C3C	3.03	0.40
14:B4:812:CLA:H2A	14:B4:812:CLA:O2A	2.20	0.40
2:B4:181:LEU:HG	14:B4:815:CLA:H43	2.03	0.40
2:B5:417:HIS:ND1	14:B5:1832:CLA:HED1	2.35	0.40
4:D1:83:TYR:CE2	4:D1:93:LEU:HG	2.56	0.40
4:D4:9:LEU:HB2	4:D4:48:VAL:HB	2.03	0.40
4:D5:28:ALA:HB2	4:D5:57:TYR:CD2	2.55	0.40
14:B3:1840:CLA:H202	6:F3:71:LEU:HD11	2.03	0.40
14:J5:101:CLA:H3A	14:J5:101:CLA:HBA2	1.68	0.40
10:L1:94:ALA:O	10:L1:98:LEU:HG	2.20	0.40
14:L4:203:CLA:HBA1	10:L5:87:LEU:CD2	2.51	0.40
10:L5:38:ARG:NH2	14:L5:204:CLA:C4C	2.84	0.40
10:L6:6:LYS:HB2	10:L6:7:PRO:HD2	2.03	0.40
11:M5:12:LEU:HB3	16:M5:101:BCR:C21	2.51	0.40
12:X4:23:ASN:ND2	14:X4:102:CLA:C4D	2.84	0.40
1:A1:248:LEU:HD12	1:A1:251:GLU:OE2	2.21	0.40
1:A1:98:SER:HB2	1:A1:113:SER:O	2.21	0.40
14:A2:1612:CLA:H3A	14:A2:1612:CLA:HBA2	1.70	0.40
14:A2:1621:CLA:O1A	14:A2:1631:CLA:HMD1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:455:SER:O	1:A2:458:LEU:HG	2.21	0.40
1:A2:420:TYR:CD2	1:A2:561:ARG:HD2	2.56	0.40
1:A3:589:VAL:HG13	2:B3:675:GLY:HA3	2.04	0.40
14:A3:828:CLA:H62	14:A3:828:CLA:H41	1.80	0.40
1:A4:221:LEU:CB	1:A4:222:PRO:HD3	2.50	0.40
1:A4:508:THR:HG22	1:A4:510:SER:H	1.86	0.40
14:A6:1612:CLA:HHC	14:A6:1612:CLA:HBB1	2.03	0.40
2:B1:290:TYR:HE2	14:B1:820:CLA:O1D	2.03	0.40
2:B1:577:SER:N	2:B1:580:ASP:OD2	2.47	0.40
2:B1:208:TRP:CE2	14:B1:815:CLA:C3D	3.04	0.40
2:B1:439:LEU:HD21	14:B1:834:CLA:HMB3	2.03	0.40
14:B1:854:CLA:O2A	14:B1:854:CLA:H2A	2.21	0.40
2:B2:496:GLY:O	2:B2:497:ASN:C	2.60	0.40
2:B3:267:LEU:HD22	14:B3:1819:CLA:HBA1	2.03	0.40
2:B3:25:ALA:HA	14:B3:1831:CLA:H42	2.03	0.40
2:B4:394:ALA:HB3	2:B4:561:TYR:HE1	1.86	0.40
2:B4:490:THR:O	2:B4:495:TYR:HA	2.22	0.40
2:B4:496:GLY:O	2:B4:497:ASN:C	2.59	0.40
2:B4:654:TRP:CH2	14:B4:801:CLA:H72	2.57	0.40
2:B5:166:TRP:CH2	14:B5:1815:CLA:HAC2	2.55	0.40
14:B5:1822:CLA:HBB1	16:B5:1845:BCR:H14C	2.03	0.40
2:B5:353:GLN:HG3	14:B5:1827:CLA:O1D	2.21	0.40
2:B5:372:ALA:HA	2:B5:600:TRP:CZ3	2.55	0.40
2:B6:553:MET:N	2:B6:554:PRO:HD3	2.35	0.40
2:B6:74:GLU:OE1	11:M6:1:MET:N	2.40	0.40
14:B6:818:CLA:H62	14:B6:818:CLA:H41	1.76	0.40
3:C4:57:CYS:HA	3:C4:58:PRO:HD3	1.77	0.40
4:D4:96:PRO:O	4:D4:97:LYS:C	2.59	0.40
5:E3:39:ARG:NH1	13:P3:24:TYR:CE2	2.90	0.40
16:B1:848:BCR:C10	6:F1:70:PHE:HE1	2.34	0.40
6:F4:100:ILE:HG21	8:J4:6:THR:CG2	2.51	0.40
1:A6:709:ASN:CB	6:F6:136:ILE:HG23	2.50	0.40
6:F6:79:TRP:CH2	6:F6:120:ALA:HA	2.56	0.40
8:J4:21:ILE:O	14:J4:101:CLA:HBB2	2.22	0.40
10:L2:65:LEU:HA	10:L2:69:ARG:HD3	2.01	0.40
10:L4:89:ALA:HB1	16:L4:206:BCR:C40	2.48	0.40
10:L5:79:LEU:HD22	10:L5:136:PHE:CD2	2.56	0.40
3:C4:11:ILE:HD12	13:P4:39:SER:C	2.41	0.40
1:A2:173:LEU:CD2	14:A2:1611:CLA:H201	2.51	0.40
14:A2:1623:CLA:HMB1	14:A2:1623:CLA:HBB1	2.03	0.40
1:A3:484:PRO:HB3	14:A3:838:CLA:HED3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:679:ALA:HB1	1:A3:738:GLY:O	2.20	0.40
14:A3:819:CLA:CBB	14:A3:819:CLA:HMB1	2.50	0.40
1:A4:207:LEU:HD23	1:A4:207:LEU:HA	1.93	0.40
1:A4:368:ILE:HG13	1:A4:401:GLY:HA3	2.03	0.40
1:A4:67:ASP:O	1:A4:71:LYS:HG3	2.20	0.40
1:A4:79:HIS:CE1	14:A4:804:CLA:CMA	3.04	0.40
14:A4:840:CLA:H62	14:A4:840:CLA:H41	1.83	0.40
1:A4:578:CYS:SG	18:A4:852:SF4:S1	3.17	0.40
1:A5:542:HIS:HB3	14:A5:836:CLA:HBB1	2.03	0.40
14:A5:821:CLA:HMB1	14:A5:821:CLA:HBB1	2.03	0.40
14:A5:826:CLA:H3A	14:A5:826:CLA:HBA2	1.87	0.40
2:B1:157:GLN:O	2:B1:161:ARG:HG3	2.21	0.40
2:B1:170:ALA:O	14:B1:825:CLA:HMD3	2.21	0.40
2:B1:235:ASN:HA	2:B1:236:PRO:HD3	1.96	0.40
2:B1:208:TRP:CD1	14:B1:815:CLA:OBD	2.74	0.40
14:B1:829:CLA:HBA2	14:B1:829:CLA:H3A	1.72	0.40
2:B2:60:VAL:HG21	14:B2:827:CLA:C1	2.47	0.40
14:B2:824:CLA:H3A	14:B2:824:CLA:HBA2	1.74	0.40
2:B3:117:SER:OG	14:B3:1810:CLA:O1D	2.23	0.40
2:B3:681:ILE:HD13	2:B3:705:ALA:N	2.36	0.40
2:B4:184:VAL:HG11	16:B4:846:BCR:H11C	2.03	0.40
2:B4:198:ILE:HB	2:B4:199:PRO:HD3	2.04	0.40
2:B4:459:GLU:HA	2:B4:460:PRO:HD3	1.86	0.40
2:B4:598:PHE:CE2	2:B4:630:LEU:HD21	2.57	0.40
14:B5:1816:CLA:HMA2	16:B5:1847:BCR:H282	2.04	0.40
2:B5:663:TRP:CZ2	2:B5:667:PHE:CZ	3.09	0.40
14:A6:1603:CLA:HMD2	2:B6:584:LEU:HB3	2.04	0.40
14:B6:804:CLA:H102	14:B6:804:CLA:H62	1.88	0.40
3:C5:2:HIS:ND1	3:C5:68:LEU:HA	2.37	0.40
4:D2:43:THR:O	4:D2:44:ALA:CB	2.69	0.40
1:A3:564:ARG:NH2	4:D3:15:GLY:HA2	2.36	0.40
4:D4:50:ARG:H	4:D4:54:ASN:HD21	1.68	0.40
5:E1:68:VAL:O	5:E1:69:ALA:O	2.39	0.40
5:E3:57:THR:CG2	13:P3:42:ALA:CA	2.97	0.40
2:B1:453:GLU:HA	6:F1:48:LEU:HD22	2.03	0.40
16:L5:201:BCR:H361	16:L5:201:BCR:H20C	1.88	0.40
1:A4:194:GLU:OE2	1:A4:194:GLU:N	2.49	0.40
1:A4:612:HIS:CE1	14:A4:835:CLA:C3C	3.04	0.40
1:A4:742:THR:HG21	14:A4:801:CLA:CHA	2.51	0.40
1:A5:593:ASP:HA	1:A5:596:PHE:HB3	2.02	0.40
1:A5:79:HIS:NE2	14:A5:805:CLA:CMA	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A6:541:ILE:HD12	14:A6:1602:CLA:H193	2.04	0.40
15:A6:1642:PQN:H212	15:A6:1642:PQN:H191	1.91	0.40
16:A6:1648:BCR:H20C	16:A6:1648:BCR:H361	1.87	0.40
1:A6:702:GLU:OE2	2:B6:552:LEU:N	2.54	0.40
14:B1:821:CLA:HBB1	16:B1:843:BCR:H14C	2.04	0.40
2:B2:377:HIS:O	2:B2:381:ILE:HG12	2.21	0.40
14:B2:827:CLA:H3A	14:B2:827:CLA:HBA2	1.72	0.40
2:B3:500:LEU:N	2:B3:501:PRO:CD	2.84	0.40
2:B4:149:LEU:O	11:M4:25:LEU:HD22	2.21	0.40
2:B4:117:SER:O	2:B4:374:LEU:HD21	2.22	0.40
2:B4:667:PHE:HB2	14:B4:805:CLA:HMC3	2.02	0.40
2:B4:216:PRO:HD3	14:B4:817:CLA:O2D	2.22	0.40
2:B4:278:ALA:HB2	14:B4:819:CLA:HBB1	2.04	0.40
2:B5:458:ILE:HD11	16:J5:105:BCR:C34	2.51	0.40
2:B6:504:LEU:HA	2:B6:507:ILE:HG22	2.02	0.40
2:B6:361:TYR:CE2	14:B6:818:CLA:O2D	2.64	0.40
16:B6:850:BCR:H20C	16:B6:850:BCR:H361	1.90	0.40
3:C1:52:ARG:O	3:C1:55:THR:HB	2.21	0.40
6:F1:103:VAL:CG1	6:F1:107:ILE:HD11	2.51	0.40
6:F2:63:PHE:C	6:F2:66:PRO:HD2	2.41	0.40
16:I4:102:BCR:HC41	14:L6:208:CLA:H201	2.04	0.40
14:B5:1835:CLA:H11	8:J5:29:PHE:CE2	2.56	0.40
14:B1:854:CLA:C20	14:L2:207:CLA:HMD1	2.50	0.40
11:M1:29:LEU:HD13	14:M1:1201:CLA:H3A	2.04	0.40
11:M2:17:LEU:HB3	11:M2:18:PRO:HD3	2.02	0.40
11:M3:17:LEU:HA	14:M3:1601:CLA:HMB3	2.02	0.40
14:A1:811:CLA:HHC	14:A1:811:CLA:HBB1	2.04	0.40
14:A1:818:CLA:CBB	14:A1:818:CLA:HMB1	2.51	0.40
14:A1:830:CLA:HMB2	14:L1:201:CLA:C1D	2.51	0.40
14:A1:832:CLA:HMD2	14:A1:833:CLA:HBB1	2.02	0.40
1:A2:557:VAL:HG11	14:A2:1623:CLA:H201	2.04	0.40
15:A2:1646:PQN:H161	15:A2:1646:PQN:H141	1.92	0.40
1:A3:293:TRP:O	1:A3:296:ASP:HB2	2.21	0.40
1:A4:220:SER:O	1:A4:224:ASN:HB2	2.21	0.40
1:A4:221:LEU:HD11	1:A4:295:SER:CA	2.52	0.40
1:A4:325:LEU:HD13	14:A4:824:CLA:HAC2	2.03	0.40
1:A5:436:HIS:HA	4:D5:14:THR:CG2	2.51	0.40
1:A5:514:GLY:HA2	1:A5:528:PRO:HB3	2.02	0.40
1:A6:683:TRP:CE3	14:A6:1602:CLA:HMA1	2.56	0.40
16:A6:1648:BCR:H381	14:B6:832:CLA:HMA1	2.04	0.40
1:A6:679:ALA:HB1	1:A6:738:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:459:GLU:HA	2:B1:460:PRO:HD3	1.90	0.40
2:B1:427:TRP:CZ2	14:B1:832:CLA:HBB1	2.56	0.40
14:B2:801:CLA:HAA2	14:B2:801:CLA:O2D	2.21	0.40
2:B3:514:LEU:CD1	14:B3:1828:CLA:CMC	2.99	0.40
2:B3:504:LEU:HA	2:B3:507:ILE:HG22	2.03	0.40
2:B3:678:GLN:HA	2:B3:681:ILE:HD12	2.02	0.40
2:B4:231:VAL:HA	2:B4:234:GLN:HG2	2.02	0.40
2:B4:529:ILE:HG21	14:B4:839:CLA:HAB	2.02	0.40
2:B5:64:LEU:HD12	2:B5:141:LEU:HD12	2.04	0.40
14:B5:1812:CLA:O2A	14:B5:1812:CLA:H2A	2.21	0.40
14:B5:1832:CLA:HBC2	16:B5:1848:BCR:H402	2.03	0.40
2:B5:504:LEU:HA	2:B5:507:ILE:HG22	2.04	0.40
2:B5:582:PHE:HZ	19:B5:1851:LMG:H341	1.86	0.40
2:B6:658:PHE:O	2:B6:662:VAL:HG23	2.22	0.40
3:C1:28:VAL:HG12	4:D1:109:ARG:HB3	2.04	0.40
2:B1:559:PHE:CE2	3:C1:67:TYR:CD2	3.10	0.40
3:C5:14:THR:O	18:C5:102:SF4:S1	2.80	0.40
3:C5:17:VAL:N	3:C5:25:LEU:HD12	2.36	0.40
5:E2:57:THR:CG2	13:P2:42:ALA:CA	2.99	0.40
6:F5:116:TRP:N	6:F5:117:PRO:CD	2.85	0.40
16:I3:102:BCR:H331	16:I3:102:BCR:C8	2.50	0.40
16:J6:1104:BCR:H341	16:J6:1104:BCR:H11C	1.95	0.40
10:L5:66:GLY:HA2	14:L5:203:CLA:CAA	2.52	0.40
10:L6:59:ILE:HD11	10:L6:135:ALA:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A1	736/755 (98%)	693 (94%)	35 (5%)	8 (1%)	16 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A2	736/755 (98%)	695 (94%)	33 (4%)	8 (1%)	16	57
1	A3	736/755 (98%)	695 (94%)	33 (4%)	8 (1%)	16	57
1	A4	736/755 (98%)	692 (94%)	35 (5%)	9 (1%)	14	55
1	A5	736/755 (98%)	695 (94%)	32 (4%)	9 (1%)	14	55
1	A6	736/755 (98%)	694 (94%)	33 (4%)	9 (1%)	14	55
2	B1	737/740 (100%)	687 (93%)	40 (5%)	10 (1%)	12	51
2	B2	737/740 (100%)	692 (94%)	35 (5%)	10 (1%)	12	51
2	B3	737/740 (100%)	695 (94%)	32 (4%)	10 (1%)	12	51
2	B4	737/740 (100%)	695 (94%)	33 (4%)	9 (1%)	14	55
2	B5	737/740 (100%)	691 (94%)	36 (5%)	10 (1%)	12	51
2	B6	737/740 (100%)	697 (95%)	30 (4%)	10 (1%)	12	51
3	C1	78/80 (98%)	72 (92%)	5 (6%)	1 (1%)	13	54
3	C2	78/80 (98%)	72 (92%)	5 (6%)	1 (1%)	13	54
3	C3	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	13	54
3	C4	78/80 (98%)	72 (92%)	5 (6%)	1 (1%)	13	54
3	C5	78/80 (98%)	64 (82%)	8 (10%)	6 (8%)	1	17
3	C6	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	13	54
4	D1	136/138 (99%)	124 (91%)	9 (7%)	3 (2%)	7	43
4	D2	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	7	43
4	D3	136/138 (99%)	126 (93%)	7 (5%)	3 (2%)	7	43
4	D4	136/138 (99%)	124 (91%)	9 (7%)	3 (2%)	7	43
4	D5	136/138 (99%)	123 (90%)	8 (6%)	5 (4%)	4	32
4	D6	136/138 (99%)	127 (93%)	6 (4%)	3 (2%)	7	43
5	E1	67/75 (89%)	56 (84%)	10 (15%)	1 (2%)	11	51
5	E2	67/75 (89%)	58 (87%)	6 (9%)	3 (4%)	3	28
5	E3	67/75 (89%)	60 (90%)	5 (8%)	2 (3%)	5	36
5	E4	67/75 (89%)	60 (90%)	5 (8%)	2 (3%)	5	36
5	E5	67/75 (89%)	56 (84%)	9 (13%)	2 (3%)	5	36
5	E6	67/75 (89%)	59 (88%)	6 (9%)	2 (3%)	5	36
6	F1	139/164 (85%)	127 (91%)	9 (6%)	3 (2%)	7	43
6	F2	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	7	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F3	139/164 (85%)	127 (91%)	9 (6%)	3 (2%)	7	43
6	F4	139/164 (85%)	127 (91%)	9 (6%)	3 (2%)	7	43
6	F5	139/164 (85%)	126 (91%)	10 (7%)	3 (2%)	7	43
6	F6	139/164 (85%)	128 (92%)	9 (6%)	2 (1%)	12	51
7	I1	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	I2	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	I3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	I4	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	I5	36/38 (95%)	25 (69%)	10 (28%)	1 (3%)	5	38
7	I6	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
8	J1	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
8	J2	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	J3	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	J4	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	J5	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
8	J6	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
9	K1	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	17
9	K2	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	17
9	K3	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	17
9	K4	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	17
9	K5	40/83 (48%)	34 (85%)	2 (5%)	4 (10%)	0	11
9	K6	40/83 (48%)	31 (78%)	7 (18%)	2 (5%)	2	26
10	L1	149/154 (97%)	138 (93%)	9 (6%)	2 (1%)	13	54
10	L2	149/154 (97%)	138 (93%)	9 (6%)	2 (1%)	13	54
10	L3	149/154 (97%)	139 (93%)	8 (5%)	2 (1%)	13	54
10	L4	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	13	54
10	L5	149/154 (97%)	116 (78%)	29 (20%)	4 (3%)	5	39
10	L6	149/154 (97%)	137 (92%)	10 (7%)	2 (1%)	13	54
11	M1	29/31 (94%)	28 (97%)	0	1 (3%)	4	34
11	M2	29/31 (94%)	28 (97%)	0	1 (3%)	4	34
11	M3	29/31 (94%)	28 (97%)	0	1 (3%)	4	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	M4	29/31 (94%)	28 (97%)	0	1 (3%)	4	34
11	M5	29/31 (94%)	25 (86%)	3 (10%)	1 (3%)	4	34
11	M6	29/31 (94%)	28 (97%)	0	1 (3%)	4	34
12	X1	27/35 (77%)	23 (85%)	3 (11%)	1 (4%)	4	32
12	X2	27/35 (77%)	23 (85%)	3 (11%)	1 (4%)	4	32
12	X3	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	4	32
12	X4	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	4	32
12	X5	27/35 (77%)	26 (96%)	0	1 (4%)	4	32
12	X6	27/35 (77%)	23 (85%)	3 (11%)	1 (4%)	4	32
13	P1	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
13	P2	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
13	P3	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
13	P4	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
13	P5	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
13	P6	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
All	All	13848/14586 (95%)	12895 (93%)	738 (5%)	215 (2%)	11	50

All (215) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A1	115	GLN
1	A1	235	ASP
1	A1	260	PHE
1	A1	578	CYS
2	B1	234	GLN
2	B1	313	LYS
2	B1	314	VAL
2	B1	480	LEU
2	B1	497	ASN
3	C1	61	PHE
6	F1	91	SER
9	K1	41	PRO
9	K1	42	GLY
11	M1	30	TYR
12	X1	10	ALA
1	A2	115	GLN
1	A2	235	ASP

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Mol	Chain	Res	Type
1	A2	260	PHE
2	B2	234	GLN
2	B2	313	LYS
2	B2	314	VAL
2	B2	480	LEU
2	B2	492	TRP
2	B2	497	ASN
2	B2	565	CYS
3	C2	62	LEU
6	F2	91	SER
9	K2	41	PRO
9	K2	42	GLY
11	M2	30	TYR
12	X2	10	ALA
1	A3	115	GLN
1	A3	235	ASP
1	A3	260	PHE
1	A3	578	CYS
2	B3	234	GLN
2	B3	313	LYS
2	B3	314	VAL
2	B3	480	LEU
2	B3	492	TRP
2	B3	497	ASN
3	C3	62	LEU
6	F3	91	SER
9	K3	41	PRO
9	K3	42	GLY
11	M3	30	TYR
12	X3	10	ALA
1	A4	115	GLN
1	A4	235	ASP
1	A4	260	PHE
1	A4	578	CYS
2	B4	234	GLN
2	B4	313	LYS
2	B4	314	VAL
2	B4	480	LEU
2	B4	492	TRP
2	B4	497	ASN
2	B4	565	CYS
3	C4	62	LEU

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Mol	Chain	Res	Type
6	F4	91	SER
9	K4	41	PRO
9	K4	42	GLY
11	M4	30	TYR
12	X4	10	ALA
1	A6	115	GLN
1	A6	235	ASP
1	A6	260	PHE
2	B6	234	GLN
2	B6	313	LYS
2	B6	314	VAL
2	B6	480	LEU
2	B6	492	TRP
2	B6	497	ASN
2	B6	565	CYS
3	C6	62	LEU
9	K6	41	PRO
9	K6	42	GLY
11	M6	30	TYR
12	X6	10	ALA
1	A5	115	GLN
1	A5	235	ASP
1	A5	260	PHE
2	B5	234	GLN
2	B5	313	LYS
2	B5	314	VAL
2	B5	480	LEU
2	B5	492	TRP
2	B5	497	ASN
2	B5	565	CYS
3	C5	14	THR
3	C5	61	PHE
3	C5	62	LEU
5	E5	55	VAL
9	K5	41	PRO
9	K5	42	GLY
10	L5	38	ARG
11	M5	30	TYR
1	A1	121	VAL
1	A1	234	LYS
1	A1	261	PHE
2	B1	492	TRP

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Mol	Chain	Res	Type
2	B1	510	GLY
6	F1	60	ALA
10	L1	106	SER
1	A2	121	VAL
1	A2	234	LYS
1	A2	261	PHE
1	A2	578	CYS
2	B2	510	GLY
4	D2	2	THR
6	F2	60	ALA
6	F2	89	ARG
1	A3	121	VAL
1	A3	234	LYS
1	A3	261	PHE
2	B3	510	GLY
2	B3	565	CYS
4	D3	2	THR
6	F3	60	ALA
6	F3	89	ARG
10	L3	104	GLY
10	L3	106	SER
1	A4	121	VAL
1	A4	234	LYS
1	A4	261	PHE
2	B4	510	GLY
4	D4	2	THR
6	F4	60	ALA
6	F4	89	ARG
10	L4	104	GLY
10	L4	106	SER
1	A6	121	VAL
1	A6	261	PHE
2	B6	510	GLY
4	D6	2	THR
6	F6	91	SER
10	L6	106	SER
1	A5	121	VAL
1	A5	261	PHE
1	A5	578	CYS
2	B5	510	GLY
3	C5	17	VAL
7	I5	5	TYR

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Mol	Chain	Res	Type
9	K5	36	SER
10	L5	60	GLY
12	X5	10	ALA
2	B1	481	LEU
2	B1	565	CYS
6	F1	89	ARG
10	L1	104	GLY
4	D2	44	ALA
10	L2	104	GLY
10	L2	106	SER
2	B3	221	LEU
2	B3	481	LEU
4	D3	44	ALA
4	D4	44	ALA
1	A6	234	LYS
1	A6	578	CYS
4	D6	44	ALA
6	F6	89	ARG
10	L6	104	GLY
1	A5	234	LYS
4	D5	3	LEU
6	F5	89	ARG
1	A1	232	ALA
4	D1	2	THR
2	B2	481	LEU
4	D2	3	LEU
1	A3	232	ALA
4	D3	3	LEU
5	E3	25	SER
2	B4	481	LEU
4	D4	3	LEU
1	A6	232	ALA
2	B6	481	LEU
5	E6	25	SER
1	A5	232	ALA
2	B5	221	LEU
2	B5	481	LEU
3	C5	15	GLN
4	D5	2	THR
6	F5	91	SER
10	L5	117	TRP
2	B1	221	LEU

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Mol	Chain	Res	Type
5	E1	55	VAL
1	A2	232	ALA
2	B2	221	LEU
5	E2	25	SER
5	E2	53	SER
5	E2	55	VAL
5	E3	55	VAL
9	K3	56	LEU
1	A4	232	ALA
5	E4	55	VAL
2	B6	221	LEU
4	D6	3	LEU
5	E6	55	VAL
3	C5	40	SER
4	D5	44	ALA
4	D5	130	PHE
10	L5	16	HIS
5	E4	53	SER
9	K4	56	LEU
4	D1	8	PRO
9	K1	56	LEU
9	K2	56	LEU
1	A5	42	PRO
9	K5	76	GLY
4	D5	7	PRO
5	E5	54	GLY
1	A4	42	PRO
6	F5	113	GLY
4	D1	16	GLY
1	A6	42	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A1	589/603 (98%)	572 (97%)	17 (3%)	45 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A2	589/603 (98%)	570 (97%)	19 (3%)	42	68
1	A3	589/603 (98%)	560 (95%)	29 (5%)	27	59
1	A4	589/603 (98%)	566 (96%)	23 (4%)	35	65
1	A5	589/603 (98%)	563 (96%)	26 (4%)	31	62
1	A6	589/603 (98%)	567 (96%)	22 (4%)	37	66
2	B1	595/597 (100%)	572 (96%)	23 (4%)	35	65
2	B2	595/597 (100%)	566 (95%)	29 (5%)	27	59
2	B3	595/597 (100%)	569 (96%)	26 (4%)	31	62
2	B4	595/597 (100%)	559 (94%)	36 (6%)	20	54
2	B5	595/597 (100%)	574 (96%)	21 (4%)	39	67
2	B6	595/597 (100%)	568 (96%)	27 (4%)	30	62
3	C1	67/67 (100%)	59 (88%)	8 (12%)	6	27
3	C2	67/67 (100%)	61 (91%)	6 (9%)	10	38
3	C3	67/67 (100%)	64 (96%)	3 (4%)	30	62
3	C4	67/67 (100%)	62 (92%)	5 (8%)	15	47
3	C5	67/67 (100%)	61 (91%)	6 (9%)	10	38
3	C6	67/67 (100%)	62 (92%)	5 (8%)	15	47
4	D1	115/115 (100%)	111 (96%)	4 (4%)	39	67
4	D2	115/115 (100%)	108 (94%)	7 (6%)	20	54
4	D3	115/115 (100%)	109 (95%)	6 (5%)	25	58
4	D4	115/115 (100%)	111 (96%)	4 (4%)	39	67
4	D5	115/115 (100%)	110 (96%)	5 (4%)	32	63
4	D6	115/115 (100%)	109 (95%)	6 (5%)	25	58
5	E1	59/64 (92%)	55 (93%)	4 (7%)	17	50
5	E2	59/64 (92%)	55 (93%)	4 (7%)	17	50
5	E3	59/64 (92%)	54 (92%)	5 (8%)	12	42
5	E4	59/64 (92%)	55 (93%)	4 (7%)	17	50
5	E5	59/64 (92%)	58 (98%)	1 (2%)	63	83
5	E6	59/64 (92%)	56 (95%)	3 (5%)	26	59
6	F1	109/128 (85%)	105 (96%)	4 (4%)	37	66
6	F2	109/128 (85%)	106 (97%)	3 (3%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F3	109/128 (85%)	106 (97%)	3 (3%)	47	71
6	F4	109/128 (85%)	107 (98%)	2 (2%)	62	82
6	F5	109/128 (85%)	108 (99%)	1 (1%)	81	90
6	F6	109/128 (85%)	107 (98%)	2 (2%)	62	82
7	I1	32/32 (100%)	31 (97%)	1 (3%)	43	69
7	I2	32/32 (100%)	29 (91%)	3 (9%)	9	36
7	I3	32/32 (100%)	31 (97%)	1 (3%)	43	69
7	I4	32/32 (100%)	30 (94%)	2 (6%)	20	52
7	I5	32/32 (100%)	30 (94%)	2 (6%)	20	52
7	I6	32/32 (100%)	31 (97%)	1 (3%)	43	69
8	J1	36/36 (100%)	34 (94%)	2 (6%)	23	56
8	J2	36/36 (100%)	34 (94%)	2 (6%)	23	56
8	J3	36/36 (100%)	34 (94%)	2 (6%)	23	56
8	J4	36/36 (100%)	34 (94%)	2 (6%)	23	56
8	J5	36/36 (100%)	34 (94%)	2 (6%)	23	56
8	J6	36/36 (100%)	34 (94%)	2 (6%)	23	56
10	L1	117/119 (98%)	106 (91%)	11 (9%)	9	36
10	L2	117/119 (98%)	110 (94%)	7 (6%)	21	54
10	L3	117/119 (98%)	106 (91%)	11 (9%)	9	36
10	L4	117/119 (98%)	106 (91%)	11 (9%)	9	36
10	L5	117/119 (98%)	108 (92%)	9 (8%)	14	46
10	L6	117/119 (98%)	108 (92%)	9 (8%)	14	46
11	M1	26/26 (100%)	25 (96%)	1 (4%)	36	65
11	M2	26/26 (100%)	25 (96%)	1 (4%)	36	65
11	M3	26/26 (100%)	24 (92%)	2 (8%)	14	46
11	M4	26/26 (100%)	25 (96%)	1 (4%)	36	65
11	M5	26/26 (100%)	25 (96%)	1 (4%)	36	65
11	M6	26/26 (100%)	24 (92%)	2 (8%)	14	46
12	X1	20/24 (83%)	19 (95%)	1 (5%)	27	59
12	X2	20/24 (83%)	19 (95%)	1 (5%)	27	59
12	X3	20/24 (83%)	19 (95%)	1 (5%)	27	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	X4	20/24 (83%)	19 (95%)	1 (5%)	27	59
12	X5	20/24 (83%)	18 (90%)	2 (10%)	8	33
12	X6	20/24 (83%)	19 (95%)	1 (5%)	27	59
13	P1	85/85 (100%)	85 (100%)	0	100	100
13	P2	85/85 (100%)	85 (100%)	0	100	100
13	P3	85/85 (100%)	85 (100%)	0	100	100
13	P4	85/85 (100%)	85 (100%)	0	100	100
13	P5	85/85 (100%)	85 (100%)	0	100	100
13	P6	85/85 (100%)	85 (100%)	0	100	100
All	All	11100/11376 (98%)	10606 (96%)	494 (4%)	30	62

All (494) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	19	ASP
1	A1	61	HIS
1	A1	145	GLN
1	A1	147	TRP
1	A1	186	LYS
1	A1	204	LEU
1	A1	210	LEU
1	A1	281	PHE
1	A1	372	GLN
1	A1	466	ARG
1	A1	477	ASP
1	A1	518	VAL
1	A1	568	ASP
1	A1	587	CYS
1	A1	632	SER
1	A1	675	LEU
1	A1	713	VAL
2	B1	53	LEU
2	B1	61	SER
2	B1	110	ASN
2	B1	125	THR
2	B1	159	LYS
2	B1	171	GLU
2	B1	213	SER
2	B1	256	PHE

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Mol	Chain	Res	Type
2	B1	318	PHE
2	B1	366	GLN
2	B1	411	LEU
2	B1	430	LEU
2	B1	446	VAL
2	B1	505	ASP
2	B1	525	VAL
2	B1	582	PHE
2	B1	589	MET
2	B1	596	VAL
2	B1	605	LEU
2	B1	632	LEU
2	B1	651	VAL
2	B1	701	ASP
2	B1	720	SER
3	C1	10	CYS
3	C1	15	GLN
3	C1	22	THR
3	C1	37	GLN
3	C1	48	VAL
3	C1	61	PHE
3	C1	63	SER
3	C1	65	ARG
4	D1	61	LYS
4	D1	73	ARG
4	D1	93	LEU
4	D1	105	VAL
5	E1	7	VAL
5	E1	25	SER
5	E1	59	ASN
5	E1	68	VAL
6	F1	1	ASP
6	F1	30	SER
6	F1	91	SER
6	F1	105	LEU
7	I1	10	LEU
8	J1	1	MET
8	J1	19	MET
10	L1	4	LEU
10	L1	22	SER
10	L1	23	ASP
10	L1	34	LEU

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Mol	Chain	Res	Type
10	L1	48	LEU
10	L1	54	HIS
10	L1	69	ARG
10	L1	71	SER
10	L1	90	THR
10	L1	107	SER
10	L1	143	LEU
11	M1	17	LEU
12	X1	8	THR
1	A2	59	ASP
1	A2	145	GLN
1	A2	147	TRP
1	A2	172	MET
1	A2	186	LYS
1	A2	210	LEU
1	A2	224	ASN
1	A2	251	GLU
1	A2	281	PHE
1	A2	324	SER
1	A2	372	GLN
1	A2	477	ASP
1	A2	516	ASP
1	A2	578	CYS
1	A2	632	SER
1	A2	647	ASN
1	A2	652	ASP
1	A2	675	LEU
1	A2	713	VAL
2	B2	61	SER
2	B2	78	GLN
2	B2	97	LYS
2	B2	109	SER
2	B2	159	LYS
2	B2	209	ASP
2	B2	256	PHE
2	B2	308	ASP
2	B2	318	PHE
2	B2	411	LEU
2	B2	412	ASP
2	B2	430	LEU
2	B2	479	THR
2	B2	482	SER

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Mol	Chain	Res	Type
2	B2	525	VAL
2	B2	538	LEU
2	B2	566	ASP
2	B2	575	ASP
2	B2	582	PHE
2	B2	589	MET
2	B2	605	LEU
2	B2	616	ASN
2	B2	621	TYR
2	B2	632	LEU
2	B2	646	THR
2	B2	648	ASN
2	B2	651	VAL
2	B2	698	ARG
2	B2	720	SER
3	C2	15	GLN
3	C2	18	ARG
3	C2	33	CYS
3	C2	45	GLU
3	C2	61	PHE
3	C2	65	ARG
4	D2	83	TYR
4	D2	93	LEU
4	D2	105	VAL
4	D2	117	ARG
4	D2	118	SER
4	D2	126	SER
4	D2	129	LYS
5	E2	7	VAL
5	E2	25	SER
5	E2	49	SER
5	E2	68	VAL
6	F2	1	ASP
6	F2	23	ASN
6	F2	24	THR
7	I2	4	SER
7	I2	8	SER
7	I2	10	LEU
8	J2	1	MET
8	J2	19	MET
10	L2	4	LEU
10	L2	48	LEU

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Mol	Chain	Res	Type
10	L2	69	ARG
10	L2	85	LEU
10	L2	108	SER
10	L2	113	THR
10	L2	134	VAL
11	M2	17	LEU
12	X2	8	THR
1	A3	19	ASP
1	A3	59	ASP
1	A3	88	SER
1	A3	108	THR
1	A3	145	GLN
1	A3	147	TRP
1	A3	195	SER
1	A3	197	LEU
1	A3	204	LEU
1	A3	210	LEU
1	A3	221	LEU
1	A3	235	ASP
1	A3	251	GLU
1	A3	277	ASP
1	A3	281	PHE
1	A3	295	SER
1	A3	349	THR
1	A3	372	GLN
1	A3	390	GLN
1	A3	433	VAL
1	A3	438	ASP
1	A3	466	ARG
1	A3	492	ASN
1	A3	516	ASP
1	A3	518	VAL
1	A3	632	SER
1	A3	675	LEU
1	A3	691	PHE
1	A3	713	VAL
2	B3	34	ASP
2	B3	53	LEU
2	B3	61	SER
2	B3	78	GLN
2	B3	97	LYS
2	B3	159	LYS

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Mol	Chain	Res	Type
2	B3	171	GLU
2	B3	182	PHE
2	B3	256	PHE
2	B3	308	ASP
2	B3	318	PHE
2	B3	396	PHE
2	B3	430	LEU
2	B3	446	VAL
2	B3	482	SER
2	B3	525	VAL
2	B3	550	SER
2	B3	582	PHE
2	B3	583	TYR
2	B3	589	MET
2	B3	611	ASN
2	B3	621	TYR
2	B3	632	LEU
2	B3	647	ASN
2	B3	648	ASN
2	B3	697	VAL
3	C3	15	GLN
3	C3	33	CYS
3	C3	40	SER
4	D3	70	GLN
4	D3	73	ARG
4	D3	88	ASP
4	D3	93	LEU
4	D3	126	SER
4	D3	129	LYS
5	E3	7	VAL
5	E3	18	ASN
5	E3	57	THR
5	E3	59	ASN
5	E3	68	VAL
6	F3	1	ASP
6	F3	24	THR
6	F3	64	LEU
7	I3	10	LEU
8	J3	1	MET
8	J3	19	MET
10	L3	4	LEU
10	L3	24	SER

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Mol	Chain	Res	Type
10	L3	34	LEU
10	L3	42	SER
10	L3	44	ILE
10	L3	48	LEU
10	L3	69	ARG
10	L3	85	LEU
10	L3	134	VAL
10	L3	143	LEU
10	L3	149	MET
11	M3	6	THR
11	M3	17	LEU
12	X3	8	THR
1	A4	59	ASP
1	A4	63	SER
1	A4	145	GLN
1	A4	147	TRP
1	A4	186	LYS
1	A4	195	SER
1	A4	204	LEU
1	A4	210	LEU
1	A4	224	ASN
1	A4	235	ASP
1	A4	281	PHE
1	A4	372	GLN
1	A4	386	ASP
1	A4	435	ARG
1	A4	447	VAL
1	A4	466	ARG
1	A4	516	ASP
1	A4	566	ILE
1	A4	579	ASP
1	A4	675	LEU
1	A4	686	SER
1	A4	713	VAL
1	A4	742	THR
2	B4	53	LEU
2	B4	61	SER
2	B4	75	GLN
2	B4	78	GLN
2	B4	94	GLN
2	B4	97	LYS
2	B4	146	SER

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Mol	Chain	Res	Type
2	B4	159	LYS
2	B4	171	GLU
2	B4	237	ASP
2	B4	256	PHE
2	B4	263	GLN
2	B4	271	ASP
2	B4	318	PHE
2	B4	327	GLU
2	B4	411	LEU
2	B4	412	ASP
2	B4	430	LEU
2	B4	444	ASP
2	B4	446	VAL
2	B4	482	SER
2	B4	485	ASP
2	B4	505	ASP
2	B4	525	VAL
2	B4	566	ASP
2	B4	574	CYS
2	B4	582	PHE
2	B4	596	VAL
2	B4	619	SER
2	B4	621	TYR
2	B4	632	LEU
2	B4	638	ILE
2	B4	648	ASN
2	B4	651	VAL
2	B4	685	VAL
2	B4	698	ARG
3	C4	10	CYS
3	C4	15	GLN
3	C4	31	ASP
3	C4	45	GLU
3	C4	61	PHE
4	D4	61	LYS
4	D4	73	ARG
4	D4	93	LEU
4	D4	117	ARG
5	E4	25	SER
5	E4	51	SER
5	E4	59	ASN
5	E4	68	VAL

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Mol	Chain	Res	Type
6	F4	24	THR
6	F4	64	LEU
7	I4	10	LEU
7	I4	13	ILE
8	J4	1	MET
8	J4	19	MET
10	L4	4	LEU
10	L4	11	ASP
10	L4	34	LEU
10	L4	42	SER
10	L4	48	LEU
10	L4	69	ARG
10	L4	85	LEU
10	L4	93	LEU
10	L4	114	SER
10	L4	115	GLU
10	L4	134	VAL
11	M4	17	LEU
12	X4	8	THR
1	A6	50	ASN
1	A6	108	THR
1	A6	145	GLN
1	A6	147	TRP
1	A6	186	LYS
1	A6	195	SER
1	A6	204	LEU
1	A6	210	LEU
1	A6	235	ASP
1	A6	251	GLU
1	A6	253	TYR
1	A6	324	SER
1	A6	349	THR
1	A6	372	GLN
1	A6	433	VAL
1	A6	463	ASP
1	A6	466	ARG
1	A6	473	ASP
1	A6	516	ASP
1	A6	632	SER
1	A6	675	LEU
1	A6	713	VAL
2	B6	61	SER

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Mol	Chain	Res	Type
2	B6	75	GLN
2	B6	78	GLN
2	B6	97	LYS
2	B6	113	ASP
2	B6	159	LYS
2	B6	165	SER
2	B6	171	GLU
2	B6	256	PHE
2	B6	263	GLN
2	B6	318	PHE
2	B6	411	LEU
2	B6	419	GLU
2	B6	430	LEU
2	B6	480	LEU
2	B6	482	SER
2	B6	525	VAL
2	B6	550	SER
2	B6	582	PHE
2	B6	583	TYR
2	B6	589	MET
2	B6	596	VAL
2	B6	632	LEU
2	B6	678	GLN
2	B6	698	ARG
2	B6	699	TRP
2	B6	720	SER
3	C6	15	GLN
3	C6	33	CYS
3	C6	40	SER
3	C6	53	CYS
3	C6	61	PHE
4	D6	23	THR
4	D6	61	LYS
4	D6	93	LEU
4	D6	105	VAL
4	D6	121	GLN
4	D6	129	LYS
5	E6	18	ASN
5	E6	57	THR
5	E6	59	ASN
6	F6	56	ARG
6	F6	133	ASP

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Mol	Chain	Res	Type
7	I6	10	LEU
8	J6	1	MET
8	J6	19	MET
10	L6	4	LEU
10	L6	22	SER
10	L6	23	ASP
10	L6	33	ASN
10	L6	48	LEU
10	L6	61	PRO
10	L6	69	ARG
10	L6	85	LEU
10	L6	134	VAL
11	M6	17	LEU
11	M6	30	TYR
12	X6	8	THR
1	A5	17	ASP
1	A5	46	THR
1	A5	59	ASP
1	A5	104	LEU
1	A5	108	THR
1	A5	145	GLN
1	A5	147	TRP
1	A5	172	MET
1	A5	186	LYS
1	A5	210	LEU
1	A5	224	ASN
1	A5	251	GLU
1	A5	277	ASP
1	A5	281	PHE
1	A5	365	SER
1	A5	372	GLN
1	A5	466	ARG
1	A5	518	VAL
1	A5	535	ASP
1	A5	538	VAL
1	A5	578	CYS
1	A5	587	CYS
1	A5	652	ASP
1	A5	667	SER
1	A5	675	LEU
1	A5	713	VAL
2	B5	61	SER

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Mol	Chain	Res	Type
2	B5	83	THR
2	B5	159	LYS
2	B5	165	SER
2	B5	171	GLU
2	B5	237	ASP
2	B5	256	PHE
2	B5	263	GLN
2	B5	318	PHE
2	B5	357	SER
2	B5	444	ASP
2	B5	446	VAL
2	B5	453	GLU
2	B5	525	VAL
2	B5	577	SER
2	B5	582	PHE
2	B5	589	MET
2	B5	592	THR
2	B5	596	VAL
2	B5	632	LEU
2	B5	651	VAL
3	C5	13	CYS
3	C5	16	CYS
3	C5	18	ARG
3	C5	22	THR
3	C5	61	PHE
3	C5	65	ARG
4	D5	33	SER
4	D5	73	ARG
4	D5	103	GLU
4	D5	105	VAL
4	D5	117	ARG
5	E5	18	ASN
6	F5	105	LEU
7	I5	8	SER
7	I5	10	LEU
8	J5	1	MET
8	J5	19	MET
10	L5	4	LEU
10	L5	22	SER
10	L5	41	LEU
10	L5	44	ILE
10	L5	48	LEU

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Mol	Chain	Res	Type
10	L5	69	ARG
10	L5	85	LEU
10	L5	107	SER
10	L5	114	SER
11	M5	17	LEU
12	X5	8	THR
12	X5	23	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (170) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	33	HIS
1	A1	145	GLN
1	A1	353	HIS
1	A1	359	ASN
1	A1	372	GLN
1	A1	390	GLN
1	A1	445	ASN
1	A1	588	GLN
1	A1	604	ASN
1	A1	647	ASN
1	A1	718	GLN
2	B1	136	GLN
2	B1	192	HIS
2	B1	261	HIS
2	B1	298	HIS
2	B1	334	HIS
2	B1	406	ASN
2	B1	494	ASN
2	B1	616	ASN
2	B1	639	ASN
2	B1	688	HIS
3	C1	37	GLN
4	D1	54	ASN
4	D1	70	GLN
4	D1	121	GLN
8	J1	39	HIS
10	L1	54	HIS
1	A2	61	HIS
1	A2	145	GLN
1	A2	353	HIS
1	A2	355	GLN

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Mol	Chain	Res	Type
1	A2	359	ASN
1	A2	372	GLN
1	A2	445	ASN
1	A2	542	HIS
1	A2	571	ASN
1	A2	647	ASN
1	A2	718	GLN
2	B2	33	HIS
2	B2	136	GLN
2	B2	261	HIS
2	B2	263	GLN
2	B2	353	GLN
2	B2	406	ASN
2	B2	616	ASN
2	B2	633	ASN
2	B2	639	ASN
2	B2	678	GLN
3	C2	15	GLN
4	D2	70	GLN
4	D2	71	GLN
4	D2	121	GLN
5	E2	18	ASN
1	A3	33	HIS
1	A3	50	ASN
1	A3	145	GLN
1	A3	192	ASN
1	A3	224	ASN
1	A3	353	HIS
1	A3	359	ASN
1	A3	372	GLN
1	A3	390	GLN
1	A3	445	ASN
1	A3	481	GLN
1	A3	483	GLN
1	A3	488	GLN
1	A3	641	GLN
2	B3	261	HIS
2	B3	336	GLN
2	B3	340	HIS
2	B3	494	ASN
2	B3	616	ASN
2	B3	639	ASN

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Mol	Chain	Res	Type
2	B3	647	ASN
2	B3	648	ASN
2	B3	678	GLN
2	B3	688	HIS
3	C3	37	GLN
4	D3	54	ASN
4	D3	127	GLN
5	E3	18	ASN
6	F3	40	GLN
6	F3	95	ASN
8	J3	39	HIS
10	L3	75	ASN
1	A4	33	HIS
1	A4	50	ASN
1	A4	145	GLN
1	A4	353	HIS
1	A4	359	ASN
1	A4	372	GLN
1	A4	445	ASN
1	A4	604	ASN
1	A4	718	GLN
2	B4	33	HIS
2	B4	78	GLN
2	B4	110	ASN
2	B4	241	HIS
2	B4	261	HIS
2	B4	263	GLN
2	B4	340	HIS
2	B4	353	GLN
2	B4	406	ASN
2	B4	591	ASN
2	B4	616	ASN
2	B4	633	ASN
2	B4	639	ASN
4	D4	54	ASN
4	D4	95	HIS
4	D4	127	GLN
5	E4	18	ASN
6	F4	95	ASN
8	J4	39	HIS
1	A6	61	HIS
1	A6	145	GLN

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Mol	Chain	Res	Type
1	A6	224	ASN
1	A6	353	HIS
1	A6	359	ASN
1	A6	372	GLN
1	A6	390	GLN
1	A6	445	ASN
1	A6	488	GLN
1	A6	718	GLN
2	B6	33	HIS
2	B6	261	HIS
2	B6	263	GLN
2	B6	336	GLN
2	B6	616	ASN
2	B6	678	GLN
2	B6	688	HIS
4	D6	54	ASN
4	D6	70	GLN
4	D6	121	GLN
4	D6	127	GLN
5	E6	18	ASN
6	F6	40	GLN
6	F6	50	HIS
10	L6	33	ASN
1	A5	145	GLN
1	A5	359	ASN
1	A5	390	GLN
1	A5	445	ASN
1	A5	539	HIS
1	A5	542	HIS
1	A5	604	ASN
1	A5	633	HIS
1	A5	718	GLN
2	B5	121	HIS
2	B5	261	HIS
2	B5	263	GLN
2	B5	340	HIS
2	B5	366	GLN
2	B5	494	ASN
2	B5	616	ASN
2	B5	639	ASN
2	B5	647	ASN
3	C5	15	GLN

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Mol	Chain	Res	Type
4	D5	54	ASN
4	D5	70	GLN
4	D5	71	GLN
4	D5	78	ASN
5	E5	18	ASN
6	F5	95	ASN
8	J5	39	HIS
12	X5	23	ASN
13	P1	92	GLN
13	P3	92	GLN
13	P4	92	GLN
13	P6	92	GLN
13	P5	92	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 774 ligands modelled in this entry, 6 are monoatomic - leaving 768 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	CLA	A1	801	-	58,73,73	1.16	5 (8%)	66,113,113	2.33	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A1	802	-	58,73,73	1.11	7 (12%)	66,113,113	1.48	9 (13%)
14	CLA	A1	803	14	52,67,73	1.24	6 (11%)	58,105,113	1.75	13 (22%)
14	CLA	A1	804	-	58,73,73	1.16	6 (10%)	66,113,113	1.47	9 (13%)
14	CLA	A1	805	-	58,73,73	1.25	7 (12%)	66,113,113	1.76	15 (22%)
14	CLA	A1	806	-	44,59,73	1.34	7 (15%)	49,96,113	1.76	9 (18%)
14	CLA	A1	807	1	58,73,73	1.17	7 (12%)	66,113,113	1.57	11 (16%)
14	CLA	A1	808	1	58,73,73	1.15	7 (12%)	66,113,113	1.59	10 (15%)
14	CLA	A1	809	-	35,53,73	1.37	7 (20%)	38,89,113	1.87	8 (21%)
14	CLA	A1	810	14	58,73,73	1.13	6 (10%)	66,113,113	1.53	10 (15%)
14	CLA	A1	811	-	47,62,73	1.34	7 (14%)	52,99,113	1.58	8 (15%)
14	CLA	A1	812	-	53,68,73	1.22	6 (11%)	60,107,113	1.61	12 (20%)
14	CLA	A1	813	-	35,53,73	1.49	7 (20%)	38,89,113	1.74	8 (21%)
14	CLA	A1	814	-	35,53,73	1.54	6 (17%)	38,89,113	1.84	11 (28%)
14	CLA	A1	815	-	42,57,73	1.33	7 (16%)	47,93,113	1.83	11 (23%)
14	CLA	A1	816	-	47,62,73	1.27	6 (12%)	52,99,113	1.70	9 (17%)
14	CLA	A1	817	-	47,62,73	1.31	8 (17%)	52,99,113	1.68	10 (19%)
14	CLA	A1	818	-	58,73,73	1.24	9 (15%)	66,113,113	1.62	12 (18%)
14	CLA	A1	819	-	54,69,73	1.30	8 (14%)	61,108,113	1.43	8 (13%)
14	CLA	A1	820	-	58,73,73	1.18	8 (13%)	66,113,113	1.51	12 (18%)
14	CLA	A1	821	-	42,57,73	1.41	7 (16%)	47,93,113	1.63	10 (21%)
14	CLA	A1	822	-	44,59,73	1.28	7 (15%)	49,96,113	1.81	12 (24%)
14	CLA	A1	823	-	52,67,73	1.21	7 (13%)	58,105,113	1.54	9 (15%)
14	CLA	A1	824	-	58,73,73	1.20	8 (13%)	66,113,113	1.50	10 (15%)
14	CLA	A1	825	-	58,73,73	1.12	8 (13%)	66,113,113	1.57	8 (12%)
14	CLA	A1	826	-	58,73,73	1.22	9 (15%)	66,113,113	1.45	9 (13%)
14	CLA	A1	827	-	58,73,73	1.11	7 (12%)	66,113,113	1.55	11 (16%)
14	CLA	A1	828	-	58,73,73	1.25	8 (13%)	66,113,113	1.64	13 (19%)
14	CLA	A1	829	-	58,73,73	1.17	7 (12%)	66,113,113	1.57	9 (13%)
14	CLA	A1	830	-	43,58,73	1.29	7 (16%)	48,95,113	1.60	10 (20%)
14	CLA	A1	831	-	58,73,73	1.06	5 (8%)	66,113,113	1.61	11 (16%)
14	CLA	A1	832	-	47,62,73	1.30	7 (14%)	52,99,113	1.68	11 (21%)
14	CLA	A1	833	1	35,53,73	1.44	7 (20%)	38,89,113	1.77	8 (21%)
14	CLA	A1	834	-	44,59,73	1.40	6 (13%)	49,96,113	2.01	13 (26%)
14	CLA	A1	835	-	58,73,73	1.16	7 (12%)	66,113,113	1.42	7 (10%)
14	CLA	A1	836	-	40,55,73	1.43	7 (17%)	45,91,113	1.84	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A1	837	-	44,59,73	1.40	6 (13%)	49,96,113	1.94	10 (20%)
14	CLA	A1	838	-	58,73,73	1.22	6 (10%)	66,113,113	1.70	15 (22%)
14	CLA	A1	839	-	58,73,73	1.11	7 (12%)	66,113,113	1.70	12 (18%)
14	CLA	A1	840	-	32,49,73	1.45	5 (15%)	34,83,113	1.64	4 (11%)
15	PQN	A1	841	-	34,34,34	2.17	7 (20%)	42,45,45	1.71	3 (7%)
16	BCR	A1	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.42	9 (16%)
16	BCR	A1	843	-	41,41,41	0.94	1 (2%)	56,56,56	1.39	9 (16%)
16	BCR	A1	844	-	41,41,41	1.06	2 (4%)	56,56,56	1.45	11 (19%)
16	BCR	A1	845	-	41,41,41	0.98	1 (2%)	56,56,56	1.35	7 (12%)
16	BCR	A1	846	-	41,41,41	0.79	1 (2%)	56,56,56	1.36	9 (16%)
16	BCR	A1	847	-	41,41,41	0.90	2 (4%)	56,56,56	1.69	16 (28%)
17	LHG	A1	848	-	48,48,48	1.22	5 (10%)	51,54,54	1.05	3 (5%)
17	LHG	A1	849	14	26,26,48	1.62	5 (19%)	29,32,54	1.42	5 (17%)
18	SF4	A1	850	-	0,12,12	0.00	-	0,24,24	0.00	-
14	CLA	A2	1601	-	35,53,73	1.55	6 (17%)	38,89,113	1.82	9 (23%)
14	CLA	A2	1602	-	58,73,73	1.14	4 (6%)	66,113,113	2.30	15 (22%)
14	CLA	A2	1603	-	58,73,73	1.13	8 (13%)	66,113,113	1.61	12 (18%)
14	CLA	A2	1604	-	58,73,73	1.15	6 (10%)	66,113,113	1.66	14 (21%)
14	CLA	A2	1605	-	58,73,73	1.11	7 (12%)	66,113,113	1.47	9 (13%)
14	CLA	A2	1606	14	52,67,73	1.22	6 (11%)	58,105,113	1.75	11 (18%)
14	CLA	A2	1607	-	58,73,73	1.17	6 (10%)	66,113,113	1.53	11 (16%)
14	CLA	A2	1608	-	58,73,73	1.22	7 (12%)	66,113,113	1.76	14 (21%)
14	CLA	A2	1609	-	44,59,73	1.33	6 (13%)	49,96,113	1.79	8 (16%)
14	CLA	A2	1610	1	58,73,73	1.17	7 (12%)	66,113,113	1.59	10 (15%)
14	CLA	A2	1611	-	58,73,73	1.14	6 (10%)	66,113,113	1.63	11 (16%)
14	CLA	A2	1612	-	35,53,73	1.35	6 (17%)	38,89,113	1.87	8 (21%)
14	CLA	A2	1613	14	58,73,73	1.13	6 (10%)	66,113,113	1.52	9 (13%)
14	CLA	A2	1614	-	47,62,73	1.35	7 (14%)	52,99,113	1.61	10 (19%)
14	CLA	A2	1615	-	53,68,73	1.24	6 (11%)	60,107,113	1.64	12 (20%)
14	CLA	A2	1616	-	35,53,73	1.44	6 (17%)	38,89,113	1.75	9 (23%)
14	CLA	A2	1617	-	35,53,73	1.52	6 (17%)	38,89,113	1.85	11 (28%)
14	CLA	A2	1618	-	42,57,73	1.34	7 (16%)	47,93,113	1.84	11 (23%)
14	CLA	A2	1619	-	47,62,73	1.26	6 (12%)	52,99,113	1.68	9 (17%)
14	CLA	A2	1620	-	47,62,73	1.31	7 (14%)	52,99,113	1.64	10 (19%)
14	CLA	A2	1621	-	58,73,73	1.23	9 (15%)	66,113,113	1.60	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A2	1622	-	54,69,73	1.30	8 (14%)	61,108,113	1.45	8 (13%)
14	CLA	A2	1623	-	58,73,73	1.16	8 (13%)	66,113,113	1.51	10 (15%)
14	CLA	A2	1624	-	42,57,73	1.40	8 (19%)	47,93,113	1.64	8 (17%)
14	CLA	A2	1625	-	44,59,73	1.29	7 (15%)	49,96,113	1.79	9 (18%)
14	CLA	A2	1626	-	52,67,73	1.20	7 (13%)	58,105,113	1.54	8 (13%)
14	CLA	A2	1627	-	58,73,73	1.20	8 (13%)	66,113,113	1.51	10 (15%)
14	CLA	A2	1628	-	58,73,73	1.11	7 (12%)	66,113,113	1.54	8 (12%)
14	CLA	A2	1629	-	58,73,73	1.21	7 (12%)	66,113,113	1.46	9 (13%)
14	CLA	A2	1630	-	58,73,73	1.08	8 (13%)	66,113,113	1.57	11 (16%)
14	CLA	A2	1631	-	58,73,73	1.24	8 (13%)	66,113,113	1.61	10 (15%)
14	CLA	A2	1632	-	58,73,73	1.15	8 (13%)	66,113,113	1.59	9 (13%)
14	CLA	A2	1633	-	43,58,73	1.27	7 (16%)	48,95,113	1.62	10 (20%)
14	CLA	A2	1634	-	58,73,73	1.22	7 (12%)	66,113,113	1.62	12 (18%)
14	CLA	A2	1635	-	58,73,73	1.06	4 (6%)	66,113,113	1.60	11 (16%)
14	CLA	A2	1636	-	47,62,73	1.27	7 (14%)	52,99,113	1.67	11 (21%)
14	CLA	A2	1637	1	35,53,73	1.43	8 (22%)	38,89,113	1.80	8 (21%)
14	CLA	A2	1638	-	44,59,73	1.35	5 (11%)	49,96,113	2.04	15 (30%)
14	CLA	A2	1639	-	58,73,73	1.15	6 (10%)	66,113,113	1.40	7 (10%)
14	CLA	A2	1640	-	40,55,73	1.41	7 (17%)	45,91,113	1.83	11 (24%)
14	CLA	A2	1641	-	58,73,73	1.15	7 (12%)	66,113,113	1.39	8 (12%)
14	CLA	A2	1642	-	44,59,73	1.42	7 (15%)	49,96,113	1.95	12 (24%)
14	CLA	A2	1643	-	58,73,73	1.22	6 (10%)	66,113,113	1.66	13 (19%)
14	CLA	A2	1644	-	58,73,73	1.10	6 (10%)	66,113,113	1.65	13 (19%)
14	CLA	A2	1645	-	32,49,73	1.43	5 (15%)	34,83,113	1.67	5 (14%)
15	PQN	A2	1646	-	34,34,34	2.18	7 (20%)	42,45,45	1.74	3 (7%)
16	BCR	A2	1647	-	41,41,41	0.99	2 (4%)	56,56,56	1.42	9 (16%)
16	BCR	A2	1648	-	41,41,41	0.92	1 (2%)	56,56,56	1.38	8 (14%)
16	BCR	A2	1649	-	41,41,41	1.04	2 (4%)	56,56,56	1.45	12 (21%)
16	BCR	A2	1650	-	41,41,41	0.98	1 (2%)	56,56,56	1.36	10 (17%)
16	BCR	A2	1651	-	41,41,41	0.77	1 (2%)	56,56,56	1.37	9 (16%)
16	BCR	A2	1652	-	41,41,41	0.84	2 (4%)	56,56,56	1.70	17 (30%)
17	LHG	A2	1653	-	48,48,48	1.20	5 (10%)	51,54,54	1.06	3 (5%)
17	LHG	A2	1654	14	26,26,48	1.60	5 (19%)	29,32,54	1.37	5 (17%)
18	SF4	A2	1655	1,2	0,12,12	0.00	-	0,24,24	0.00	-
14	CLA	A3	801	-	58,73,73	1.15	5 (8%)	66,113,113	2.38	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A3	802	-	58,73,73	1.13	8 (13%)	66,113,113	1.63	12 (18%)
14	CLA	A3	803	-	58,73,73	1.09	7 (12%)	66,113,113	1.48	9 (13%)
14	CLA	A3	804	14	52,67,73	1.22	6 (11%)	58,105,113	1.72	11 (18%)
14	CLA	A3	805	-	58,73,73	1.14	7 (12%)	66,113,113	1.54	11 (16%)
14	CLA	A3	806	-	58,73,73	1.23	7 (12%)	66,113,113	1.72	13 (19%)
14	CLA	A3	807	-	44,59,73	1.31	7 (15%)	49,96,113	1.76	8 (16%)
14	CLA	A3	808	1	58,73,73	1.17	7 (12%)	66,113,113	1.56	11 (16%)
14	CLA	A3	809	1	58,73,73	1.14	7 (12%)	66,113,113	1.58	10 (15%)
14	CLA	A3	810	-	35,53,73	1.34	6 (17%)	38,89,113	1.81	8 (21%)
14	CLA	A3	811	14	58,73,73	1.12	6 (10%)	66,113,113	1.57	11 (16%)
14	CLA	A3	812	-	47,62,73	1.33	7 (14%)	52,99,113	1.60	9 (17%)
14	CLA	A3	813	-	53,68,73	1.23	6 (11%)	60,107,113	1.61	12 (20%)
14	CLA	A3	814	-	35,53,73	1.39	6 (17%)	38,89,113	1.76	9 (23%)
14	CLA	A3	815	-	35,53,73	1.51	6 (17%)	38,89,113	1.85	10 (26%)
14	CLA	A3	816	-	42,57,73	1.31	7 (16%)	47,93,113	1.86	13 (27%)
14	CLA	A3	817	-	47,62,73	1.28	6 (12%)	52,99,113	1.69	9 (17%)
14	CLA	A3	818	-	47,62,73	1.30	8 (17%)	52,99,113	1.66	11 (21%)
14	CLA	A3	819	-	58,73,73	1.22	8 (13%)	66,113,113	1.64	12 (18%)
14	CLA	A3	820	-	54,69,73	1.28	8 (14%)	61,108,113	1.48	10 (16%)
14	CLA	A3	821	-	58,73,73	1.17	8 (13%)	66,113,113	1.52	12 (18%)
14	CLA	A3	822	-	42,57,73	1.41	8 (19%)	47,93,113	1.63	10 (21%)
14	CLA	A3	823	-	44,59,73	1.28	7 (15%)	49,96,113	1.82	10 (20%)
14	CLA	A3	824	-	52,67,73	1.18	7 (13%)	58,105,113	1.57	8 (13%)
14	CLA	A3	825	-	58,73,73	1.18	8 (13%)	66,113,113	1.48	10 (15%)
14	CLA	A3	826	-	58,73,73	1.11	7 (12%)	66,113,113	1.59	11 (16%)
14	CLA	A3	827	-	58,73,73	1.20	7 (12%)	66,113,113	1.44	9 (13%)
14	CLA	A3	828	-	58,73,73	1.08	6 (10%)	66,113,113	1.56	11 (16%)
14	CLA	A3	829	-	58,73,73	1.22	8 (13%)	66,113,113	1.61	10 (15%)
14	CLA	A3	830	-	58,73,73	1.16	8 (13%)	66,113,113	1.57	9 (13%)
14	CLA	A3	831	-	43,58,73	1.26	7 (16%)	48,95,113	1.60	10 (20%)
14	CLA	A3	832	-	58,73,73	1.21	8 (13%)	66,113,113	1.61	11 (16%)
14	CLA	A3	833	-	58,73,73	1.04	5 (8%)	66,113,113	1.63	12 (18%)
14	CLA	A3	834	-	58,73,73	1.08	7 (12%)	66,113,113	1.65	10 (15%)
14	CLA	A3	835	-	47,62,73	1.29	7 (14%)	52,99,113	1.67	11 (21%)
14	CLA	A3	836	1	35,53,73	1.45	7 (20%)	38,89,113	1.85	10 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A3	837	-	44,59,73	1.37	6 (13%)	49,96,113	2.04	13 (26%)
14	CLA	A3	838	-	58,73,73	1.15	6 (10%)	66,113,113	1.46	10 (15%)
14	CLA	A3	839	-	40,55,73	1.39	7 (17%)	45,91,113	1.89	10 (22%)
14	CLA	A3	840	-	58,73,73	1.15	8 (13%)	66,113,113	1.38	8 (12%)
14	CLA	A3	841	-	44,59,73	1.38	6 (13%)	49,96,113	1.95	12 (24%)
14	CLA	A3	842	-	58,73,73	1.22	6 (10%)	66,113,113	1.66	13 (19%)
14	CLA	A3	843	-	58,73,73	1.07	6 (10%)	66,113,113	1.69	13 (19%)
14	CLA	A3	844	-	32,49,73	1.41	5 (15%)	34,83,113	1.65	5 (14%)
14	CLA	A3	845	17	45,60,73	1.36	8 (17%)	50,97,113	1.79	12 (24%)
15	PQN	A3	846	-	34,34,34	2.17	7 (20%)	42,45,45	1.71	3 (7%)
16	BCR	A3	847	-	41,41,41	0.99	2 (4%)	56,56,56	1.44	9 (16%)
16	BCR	A3	848	-	41,41,41	0.89	1 (2%)	56,56,56	1.39	7 (12%)
16	BCR	A3	849	-	41,41,41	1.04	2 (4%)	56,56,56	1.45	11 (19%)
16	BCR	A3	850	-	41,41,41	0.95	1 (2%)	56,56,56	1.38	10 (17%)
16	BCR	A3	851	-	41,41,41	0.76	1 (2%)	56,56,56	1.37	9 (16%)
16	BCR	A3	852	-	41,41,41	0.84	2 (4%)	56,56,56	1.70	17 (30%)
17	LHG	A3	853	-	48,48,48	1.17	5 (10%)	51,54,54	1.03	3 (5%)
17	LHG	A3	854	14	26,26,48	1.59	5 (19%)	29,32,54	1.42	5 (17%)
18	SF4	A3	855	-	0,12,12	0.00	-	0,24,24	0.00	-
16	BCR	A3	856	-	41,41,41	0.72	0	56,56,56	1.27	8 (14%)
14	CLA	A4	801	-	58,73,73	1.17	6 (10%)	66,113,113	2.35	15 (22%)
14	CLA	A4	802	-	58,73,73	1.13	7 (12%)	66,113,113	1.49	9 (13%)
14	CLA	A4	803	14	52,67,73	1.23	6 (11%)	58,105,113	1.74	12 (20%)
14	CLA	A4	804	-	58,73,73	1.18	6 (10%)	66,113,113	1.52	10 (15%)
14	CLA	A4	805	-	58,73,73	1.25	7 (12%)	66,113,113	1.79	14 (21%)
14	CLA	A4	806	-	44,59,73	1.36	6 (13%)	49,96,113	1.80	9 (18%)
14	CLA	A4	807	1	58,73,73	1.17	8 (13%)	66,113,113	1.60	11 (16%)
14	CLA	A4	808	1	58,73,73	1.16	7 (12%)	66,113,113	1.59	11 (16%)
14	CLA	A4	809	-	35,53,73	1.36	6 (17%)	38,89,113	1.84	8 (21%)
14	CLA	A4	810	14	58,73,73	1.14	7 (12%)	66,113,113	1.54	10 (15%)
14	CLA	A4	811	-	47,62,73	1.35	7 (14%)	52,99,113	1.61	10 (19%)
14	CLA	A4	812	-	53,68,73	1.25	7 (13%)	60,107,113	1.59	12 (20%)
14	CLA	A4	813	-	35,53,73	1.47	7 (20%)	38,89,113	1.75	9 (23%)
14	CLA	A4	814	-	35,53,73	1.56	6 (17%)	38,89,113	1.86	11 (28%)
14	CLA	A4	815	-	42,57,73	1.34	8 (19%)	47,93,113	1.82	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A4	816	-	47,62,73	1.28	6 (12%)	52,99,113	1.69	9 (17%)
14	CLA	A4	817	-	47,62,73	1.32	7 (14%)	52,99,113	1.67	11 (21%)
14	CLA	A4	818	-	58,73,73	1.25	10 (17%)	66,113,113	1.60	11 (16%)
14	CLA	A4	819	-	54,69,73	1.31	8 (14%)	61,108,113	1.47	8 (13%)
14	CLA	A4	820	-	58,73,73	1.18	8 (13%)	66,113,113	1.52	11 (16%)
14	CLA	A4	821	-	42,57,73	1.42	7 (16%)	47,93,113	1.65	9 (19%)
14	CLA	A4	822	-	44,59,73	1.30	7 (15%)	49,96,113	1.81	9 (18%)
14	CLA	A4	823	-	52,67,73	1.22	7 (13%)	58,105,113	1.55	8 (13%)
14	CLA	A4	824	-	58,73,73	1.21	8 (13%)	66,113,113	1.46	9 (13%)
14	CLA	A4	825	-	58,73,73	1.12	6 (10%)	66,113,113	1.57	9 (13%)
14	CLA	A4	826	-	58,73,73	1.22	7 (12%)	66,113,113	1.46	9 (13%)
14	CLA	A4	827	-	58,73,73	1.10	6 (10%)	66,113,113	1.57	10 (15%)
14	CLA	A4	828	-	58,73,73	1.25	8 (13%)	66,113,113	1.64	9 (13%)
14	CLA	A4	829	-	58,73,73	1.17	8 (13%)	66,113,113	1.56	8 (12%)
14	CLA	A4	830	-	43,58,73	1.29	7 (16%)	48,95,113	1.61	10 (20%)
14	CLA	A4	831	-	58,73,73	1.23	8 (13%)	66,113,113	1.64	12 (18%)
14	CLA	A4	832	-	58,73,73	1.07	6 (10%)	66,113,113	1.59	11 (16%)
14	CLA	A4	833	-	47,62,73	1.29	7 (14%)	52,99,113	1.65	9 (17%)
14	CLA	A4	834	1	35,53,73	1.45	7 (20%)	38,89,113	1.83	9 (23%)
14	CLA	A4	835	-	44,59,73	1.40	7 (15%)	49,96,113	2.02	13 (26%)
14	CLA	A4	836	-	58,73,73	1.17	7 (12%)	66,113,113	1.38	6 (9%)
14	CLA	A4	837	-	40,55,73	1.40	7 (17%)	45,91,113	1.85	10 (22%)
14	CLA	A4	838	-	58,73,73	1.15	8 (13%)	66,113,113	1.39	8 (12%)
14	CLA	A4	839	-	44,59,73	1.40	7 (15%)	49,96,113	1.94	9 (18%)
14	CLA	A4	840	-	58,73,73	1.22	6 (10%)	66,113,113	1.69	14 (21%)
14	CLA	A4	841	-	58,73,73	1.09	6 (10%)	66,113,113	1.68	14 (21%)
14	CLA	A4	842	-	32,49,73	1.44	5 (15%)	34,83,113	1.69	5 (14%)
15	PQN	A4	843	-	34,34,34	2.19	7 (20%)	42,45,45	1.74	3 (7%)
16	BCR	A4	844	-	41,41,41	1.02	2 (4%)	56,56,56	1.43	9 (16%)
16	BCR	A4	845	-	41,41,41	0.94	1 (2%)	56,56,56	1.40	8 (14%)
16	BCR	A4	846	-	41,41,41	1.07	2 (4%)	56,56,56	1.45	12 (21%)
16	BCR	A4	847	-	41,41,41	0.97	1 (2%)	56,56,56	1.35	9 (16%)
16	BCR	A4	848	-	41,41,41	0.80	1 (2%)	56,56,56	1.36	9 (16%)
16	BCR	A4	849	-	41,41,41	0.88	2 (4%)	56,56,56	1.70	16 (28%)
17	LHG	A4	850	-	48,48,48	1.20	5 (10%)	51,54,54	1.06	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LHG	A4	851	14	26,26,48	1.64	5 (19%)	29,32,54	1.38	5 (17%)
18	SF4	A4	852	1,2	0,12,12	0.00	-	0,24,24	0.00	-
14	CLA	A4	853	-	35,53,73	1.50	7 (20%)	38,89,113	1.83	9 (23%)
14	CLA	A5	801	-	58,73,73	1.16	5 (8%)	66,113,113	2.33	14 (21%)
14	CLA	A5	802	-	58,73,73	1.14	8 (13%)	66,113,113	1.62	14 (21%)
14	CLA	A5	803	-	58,73,73	1.11	8 (13%)	66,113,113	1.48	10 (15%)
14	CLA	A5	804	14	52,67,73	1.22	6 (11%)	58,105,113	1.75	12 (20%)
14	CLA	A5	805	-	58,73,73	1.15	6 (10%)	66,113,113	1.51	11 (16%)
14	CLA	A5	806	-	58,73,73	1.24	7 (12%)	66,113,113	1.77	16 (24%)
14	CLA	A5	807	-	44,59,73	1.31	7 (15%)	49,96,113	1.80	9 (18%)
14	CLA	A5	808	1	58,73,73	1.15	7 (12%)	66,113,113	1.57	10 (15%)
14	CLA	A5	809	-	58,73,73	1.13	6 (10%)	66,113,113	1.60	11 (16%)
14	CLA	A5	810	-	35,53,73	1.34	6 (17%)	38,89,113	1.87	8 (21%)
14	CLA	A5	811	14	58,73,73	1.15	7 (12%)	66,113,113	1.55	9 (13%)
14	CLA	A5	812	-	47,62,73	1.32	7 (14%)	52,99,113	1.58	8 (15%)
14	CLA	A5	813	-	53,68,73	1.22	7 (13%)	60,107,113	1.58	11 (18%)
14	CLA	A5	814	-	35,53,73	1.44	7 (20%)	38,89,113	1.77	8 (21%)
14	CLA	A5	815	-	35,53,73	1.53	6 (17%)	38,89,113	1.89	10 (26%)
14	CLA	A5	816	-	42,57,73	1.34	8 (19%)	47,93,113	1.85	12 (25%)
14	CLA	A5	817	-	47,62,73	1.25	6 (12%)	52,99,113	1.69	9 (17%)
14	CLA	A5	818	-	47,62,73	1.31	7 (14%)	52,99,113	1.67	11 (21%)
14	CLA	A5	819	-	58,73,73	1.21	7 (12%)	66,113,113	1.63	12 (18%)
14	CLA	A5	820	-	54,69,73	1.29	8 (14%)	61,108,113	1.46	9 (14%)
14	CLA	A5	821	-	58,73,73	1.19	8 (13%)	66,113,113	1.55	11 (16%)
14	CLA	A5	822	-	42,57,73	1.41	8 (19%)	47,93,113	1.65	10 (21%)
14	CLA	A5	823	-	44,59,73	1.29	7 (15%)	49,96,113	1.81	8 (16%)
14	CLA	A5	824	-	52,67,73	1.20	7 (13%)	58,105,113	1.55	9 (15%)
14	CLA	A5	825	-	58,73,73	1.21	8 (13%)	66,113,113	1.48	8 (12%)
14	CLA	A5	826	-	58,73,73	1.11	6 (10%)	66,113,113	1.57	8 (12%)
14	CLA	A5	827	-	58,73,73	1.20	7 (12%)	66,113,113	1.46	8 (12%)
14	CLA	A5	828	-	58,73,73	1.11	7 (12%)	66,113,113	1.52	11 (16%)
14	CLA	A5	829	-	58,73,73	1.23	8 (13%)	66,113,113	1.62	8 (12%)
14	CLA	A5	830	-	58,73,73	1.16	8 (13%)	66,113,113	1.55	8 (12%)
14	CLA	A5	831	-	43,58,73	1.28	7 (16%)	48,95,113	1.63	9 (18%)
14	CLA	A5	832	-	58,73,73	1.24	7 (12%)	66,113,113	1.59	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A5	833	-	58,73,73	1.05	6 (10%)	66,113,113	1.60	12 (18%)
14	CLA	A5	834	-	47,62,73	1.29	7 (14%)	52,99,113	1.67	10 (19%)
14	CLA	A5	835	1	35,53,73	1.42	7 (20%)	38,89,113	1.84	10 (26%)
14	CLA	A5	836	-	44,59,73	1.35	6 (13%)	49,96,113	2.04	13 (26%)
14	CLA	A5	837	-	58,73,73	1.15	7 (12%)	66,113,113	1.40	6 (9%)
14	CLA	A5	838	-	40,55,73	1.41	7 (17%)	45,91,113	1.87	12 (26%)
14	CLA	A5	839	-	58,73,73	1.17	8 (13%)	66,113,113	1.43	8 (12%)
14	CLA	A5	840	-	44,59,73	1.38	6 (13%)	49,96,113	1.96	11 (22%)
14	CLA	A5	841	-	58,73,73	1.22	6 (10%)	66,113,113	1.70	14 (21%)
14	CLA	A5	842	-	58,73,73	1.10	7 (12%)	66,113,113	1.71	13 (19%)
14	CLA	A5	843	17	45,60,73	1.36	8 (17%)	50,97,113	1.81	12 (24%)
15	PQN	A5	844	-	34,34,34	2.18	7 (20%)	42,45,45	1.71	3 (7%)
16	BCR	A5	845	-	41,41,41	0.99	2 (4%)	56,56,56	1.43	9 (16%)
16	BCR	A5	846	-	41,41,41	0.90	1 (2%)	56,56,56	1.37	8 (14%)
16	BCR	A5	847	-	41,41,41	1.04	2 (4%)	56,56,56	1.43	10 (17%)
16	BCR	A5	848	-	41,41,41	0.95	1 (2%)	56,56,56	1.35	9 (16%)
16	BCR	A5	849	-	41,41,41	0.77	1 (2%)	56,56,56	1.35	8 (14%)
16	BCR	A5	850	-	41,41,41	0.85	2 (4%)	56,56,56	1.70	16 (28%)
17	LHG	A5	851	-	48,48,48	1.21	5 (10%)	51,54,54	1.07	3 (5%)
17	LHG	A5	852	14	26,26,48	1.61	5 (19%)	29,32,54	1.43	5 (17%)
16	BCR	A5	853	-	41,41,41	0.74	0	56,56,56	1.27	7 (12%)
18	SF4	A5	854	1	0,12,12	0.00	-	0,24,24	0.00	-
14	CLA	A6	1601	-	35,53,73	1.53	7 (20%)	38,89,113	1.87	9 (23%)
14	CLA	A6	1602	-	58,73,73	1.15	5 (8%)	66,113,113	2.33	14 (21%)
14	CLA	A6	1603	-	58,73,73	1.14	6 (10%)	66,113,113	1.62	13 (19%)
14	CLA	A6	1604	14	52,67,73	1.21	6 (11%)	58,105,113	1.74	11 (18%)
14	CLA	A6	1605	-	58,73,73	1.17	7 (12%)	66,113,113	1.54	11 (16%)
14	CLA	A6	1606	-	58,73,73	1.22	7 (12%)	66,113,113	1.74	14 (21%)
14	CLA	A6	1607	-	44,59,73	1.31	6 (13%)	49,96,113	1.75	8 (16%)
14	CLA	A6	1608	1	58,73,73	1.16	7 (12%)	66,113,113	1.57	10 (15%)
14	CLA	A6	1609	-	58,73,73	1.12	6 (10%)	66,113,113	1.58	10 (15%)
14	CLA	A6	1610	-	35,53,73	1.34	6 (17%)	38,89,113	1.87	8 (21%)
14	CLA	A6	1611	14	58,73,73	1.14	7 (12%)	66,113,113	1.52	9 (13%)
14	CLA	A6	1612	-	47,62,73	1.32	7 (14%)	52,99,113	1.59	9 (17%)
14	CLA	A6	1613	-	53,68,73	1.25	7 (13%)	60,107,113	1.58	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A6	1614	-	35,53,73	1.45	8 (22%)	38,89,113	1.75	8 (21%)
14	CLA	A6	1615	-	35,53,73	1.50	6 (17%)	38,89,113	1.85	10 (26%)
14	CLA	A6	1616	-	42,57,73	1.33	7 (16%)	47,93,113	1.85	11 (23%)
14	CLA	A6	1617	-	47,62,73	1.26	6 (12%)	52,99,113	1.70	9 (17%)
14	CLA	A6	1618	-	47,62,73	1.29	8 (17%)	52,99,113	1.67	9 (17%)
14	CLA	A6	1619	-	58,73,73	1.23	8 (13%)	66,113,113	1.64	12 (18%)
14	CLA	A6	1620	-	54,69,73	1.29	8 (14%)	61,108,113	1.45	8 (13%)
14	CLA	A6	1621	-	58,73,73	1.18	8 (13%)	66,113,113	1.54	11 (16%)
14	CLA	A6	1622	-	42,57,73	1.40	8 (19%)	47,93,113	1.62	9 (19%)
14	CLA	A6	1623	-	44,59,73	1.29	7 (15%)	49,96,113	1.78	9 (18%)
14	CLA	A6	1624	-	52,67,73	1.22	7 (13%)	58,105,113	1.57	9 (15%)
14	CLA	A6	1625	-	58,73,73	1.16	8 (13%)	66,113,113	1.50	9 (13%)
14	CLA	A6	1626	-	58,73,73	1.09	7 (12%)	66,113,113	1.58	9 (13%)
14	CLA	A6	1627	-	58,73,73	1.20	7 (12%)	66,113,113	1.44	8 (12%)
14	CLA	A6	1628	-	58,73,73	1.08	7 (12%)	66,113,113	1.55	11 (16%)
14	CLA	A6	1629	-	58,73,73	1.25	9 (15%)	66,113,113	1.60	11 (16%)
14	CLA	A6	1630	-	58,73,73	1.16	8 (13%)	66,113,113	1.59	8 (12%)
14	CLA	A6	1631	-	43,58,73	1.28	7 (16%)	48,95,113	1.63	9 (18%)
14	CLA	A6	1632	-	58,73,73	1.06	6 (10%)	66,113,113	1.62	12 (18%)
14	CLA	A6	1633	-	58,73,73	1.08	7 (12%)	66,113,113	1.65	11 (16%)
14	CLA	A6	1634	-	47,62,73	1.30	7 (14%)	52,99,113	1.69	10 (19%)
14	CLA	A6	1635	1	35,53,73	1.44	7 (20%)	38,89,113	1.83	9 (23%)
14	CLA	A6	1636	-	44,59,73	1.38	6 (13%)	49,96,113	2.07	15 (30%)
14	CLA	A6	1637	-	58,73,73	1.16	6 (10%)	66,113,113	1.42	9 (13%)
14	CLA	A6	1638	-	40,55,73	1.39	7 (17%)	45,91,113	1.92	11 (24%)
14	CLA	A6	1639	-	44,59,73	1.35	6 (13%)	49,96,113	1.97	11 (22%)
14	CLA	A6	1640	-	58,73,73	1.20	6 (10%)	66,113,113	1.68	14 (21%)
14	CLA	A6	1641	-	32,49,73	1.42	5 (15%)	34,83,113	1.64	5 (14%)
15	PQN	A6	1642	-	34,34,34	2.17	7 (20%)	42,45,45	1.71	3 (7%)
16	BCR	A6	1643	-	41,41,41	1.00	2 (4%)	56,56,56	1.44	9 (16%)
16	BCR	A6	1644	-	41,41,41	0.91	1 (2%)	56,56,56	1.36	9 (16%)
16	BCR	A6	1645	-	41,41,41	1.04	2 (4%)	56,56,56	1.46	11 (19%)
16	BCR	A6	1646	-	41,41,41	0.98	1 (2%)	56,56,56	1.34	10 (17%)
16	BCR	A6	1647	-	41,41,41	0.77	1 (2%)	56,56,56	1.37	8 (14%)
16	BCR	A6	1648	-	41,41,41	0.86	2 (4%)	56,56,56	1.72	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LHG	A6	1649	-	48,48,48	1.19	5 (10%)	51,54,54	1.06	3 (5%)
17	LHG	A6	1650	14	26,26,48	1.60	5 (19%)	29,32,54	1.44	4 (13%)
14	CLA	A6	1651	-	58,73,73	1.16	10 (17%)	66,113,113	1.83	14 (21%)
16	BCR	A6	1652	-	41,41,41	0.75	0	56,56,56	1.28	9 (16%)
14	CLA	B1	801	-	58,73,73	1.16	9 (15%)	66,113,113	1.67	12 (18%)
14	CLA	B1	802	-	58,73,73	1.15	6 (10%)	66,113,113	1.63	13 (19%)
14	CLA	B1	803	-	58,73,73	1.15	7 (12%)	66,113,113	1.43	8 (12%)
14	CLA	B1	804	-	58,73,73	1.21	9 (15%)	66,113,113	1.62	12 (18%)
14	CLA	B1	805	-	58,73,73	1.17	9 (15%)	66,113,113	1.80	14 (21%)
14	CLA	B1	806	-	58,73,73	1.24	10 (17%)	66,113,113	1.35	11 (16%)
14	CLA	B1	807	-	58,73,73	1.21	7 (12%)	66,113,113	1.62	10 (15%)
14	CLA	B1	808	-	58,73,73	1.13	8 (13%)	66,113,113	1.47	10 (15%)
14	CLA	B1	809	-	58,73,73	1.10	8 (13%)	66,113,113	1.52	7 (10%)
14	CLA	B1	810	-	58,73,73	1.05	5 (8%)	66,113,113	1.73	11 (16%)
14	CLA	B1	811	-	58,73,73	1.08	7 (12%)	66,113,113	1.72	13 (19%)
14	CLA	B1	812	-	35,53,73	1.38	7 (20%)	38,89,113	1.75	6 (15%)
14	CLA	B1	813	-	35,53,73	1.52	6 (17%)	38,89,113	1.75	9 (23%)
14	CLA	B1	814	-	58,73,73	1.18	6 (10%)	66,113,113	1.57	11 (16%)
14	CLA	B1	815	-	58,73,73	1.18	7 (12%)	66,113,113	1.61	8 (12%)
14	CLA	B1	816	-	35,53,73	1.34	5 (14%)	38,89,113	1.92	8 (21%)
14	CLA	B1	817	-	48,63,73	1.34	7 (14%)	54,101,113	1.72	9 (16%)
14	CLA	B1	818	-	52,67,73	1.23	7 (13%)	58,105,113	1.59	11 (18%)
14	CLA	B1	819	-	53,68,73	1.30	8 (15%)	60,107,113	1.72	12 (20%)
14	CLA	B1	820	-	58,73,73	1.19	8 (13%)	66,113,113	1.54	10 (15%)
14	CLA	B1	821	-	40,55,73	1.48	7 (17%)	45,91,113	1.78	11 (24%)
14	CLA	B1	822	-	35,53,73	1.45	6 (17%)	38,89,113	1.74	9 (23%)
14	CLA	B1	823	-	48,63,73	1.41	7 (14%)	54,101,113	1.61	10 (18%)
14	CLA	B1	824	-	35,53,73	1.40	7 (20%)	38,89,113	1.71	7 (18%)
14	CLA	B1	825	-	47,62,73	1.39	10 (21%)	52,99,113	1.68	10 (19%)
14	CLA	B1	826	-	39,54,73	1.39	7 (17%)	44,90,113	1.82	9 (20%)
14	CLA	B1	827	-	58,73,73	1.25	7 (12%)	66,113,113	1.62	17 (25%)
14	CLA	B1	828	-	58,73,73	1.20	7 (12%)	66,113,113	1.73	13 (19%)
14	CLA	B1	829	-	58,73,73	1.21	8 (13%)	66,113,113	1.69	10 (15%)
14	CLA	B1	830	-	58,73,73	1.29	8 (13%)	66,113,113	1.69	12 (18%)
14	CLA	B1	831	-	35,53,73	1.40	7 (20%)	38,89,113	1.59	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B1	832	-	42,57,73	1.31	7 (16%)	47,93,113	1.63	8 (17%)
14	CLA	B1	833	-	58,73,73	1.18	8 (13%)	66,113,113	1.51	10 (15%)
14	CLA	B1	834	-	51,66,73	1.41	7 (13%)	57,104,113	1.65	10 (17%)
14	CLA	B1	835	-	35,53,73	1.49	6 (17%)	38,89,113	1.72	6 (15%)
14	CLA	B1	836	-	35,53,73	1.43	8 (22%)	38,89,113	1.74	7 (18%)
14	CLA	B1	837	-	35,53,73	1.48	7 (20%)	38,89,113	1.79	8 (21%)
14	CLA	B1	838	-	53,68,73	1.31	7 (13%)	60,107,113	1.48	9 (15%)
14	CLA	B1	839	-	58,73,73	1.23	8 (13%)	66,113,113	1.44	10 (15%)
14	CLA	B1	840	-	40,55,73	1.27	9 (22%)	45,91,113	1.85	10 (22%)
14	CLA	B1	841	-	58,73,73	1.11	7 (12%)	66,113,113	1.59	8 (12%)
15	PQN	B1	842	-	34,34,34	2.14	8 (23%)	42,45,45	1.51	4 (9%)
16	BCR	B1	843	-	41,41,41	1.17	3 (7%)	56,56,56	1.51	10 (17%)
16	BCR	B1	844	-	41,41,41	1.20	4 (9%)	56,56,56	1.67	14 (25%)
16	BCR	B1	845	-	41,41,41	0.95	3 (7%)	56,56,56	1.55	13 (23%)
16	BCR	B1	846	-	25,25,41	0.92	0	33,33,56	1.34	6 (18%)
16	BCR	B1	847	-	41,41,41	0.84	0	56,56,56	1.41	12 (21%)
16	BCR	B1	848	-	41,41,41	0.76	1 (2%)	56,56,56	1.55	12 (21%)
16	BCR	B1	849	-	41,41,41	0.77	0	56,56,56	1.26	8 (14%)
19	LMG	B1	850	-	55,55,55	0.86	3 (5%)	63,63,63	1.03	3 (4%)
17	LHG	B1	851	-	22,22,48	1.82	5 (22%)	25,28,54	1.09	1 (4%)
16	BCR	B1	852	-	41,41,41	1.06	3 (7%)	56,56,56	1.37	8 (14%)
14	CLA	B1	853	17	45,60,73	1.38	9 (20%)	50,97,113	1.80	12 (24%)
14	CLA	B1	854	2	58,73,73	1.12	6 (10%)	66,113,113	1.70	13 (19%)
14	CLA	B2	801	-	58,73,73	1.19	9 (15%)	66,113,113	1.61	13 (19%)
14	CLA	B2	802	-	58,73,73	1.16	9 (15%)	66,113,113	1.82	14 (21%)
14	CLA	B2	803	-	58,73,73	1.22	9 (15%)	66,113,113	1.36	9 (13%)
14	CLA	B2	804	-	58,73,73	1.19	7 (12%)	66,113,113	1.67	9 (13%)
14	CLA	B2	805	-	58,73,73	1.13	8 (13%)	66,113,113	1.52	9 (13%)
14	CLA	B2	806	-	58,73,73	1.11	8 (13%)	66,113,113	1.53	7 (10%)
14	CLA	B2	807	-	58,73,73	1.06	5 (8%)	66,113,113	1.72	10 (15%)
14	CLA	B2	808	2	58,73,73	1.08	7 (12%)	66,113,113	1.74	11 (16%)
14	CLA	B2	809	2	58,73,73	1.10	6 (10%)	66,113,113	1.68	13 (19%)
14	CLA	B2	810	-	35,53,73	1.35	7 (20%)	38,89,113	1.78	6 (15%)
14	CLA	B2	811	-	35,53,73	1.51	6 (17%)	38,89,113	1.71	9 (23%)
14	CLA	B2	812	-	58,73,73	1.17	7 (12%)	66,113,113	1.63	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B2	813	-	58,73,73	1.17	7 (12%)	66,113,113	1.57	7 (10%)
14	CLA	B2	814	-	35,53,73	1.31	6 (17%)	38,89,113	1.96	8 (21%)
14	CLA	B2	815	-	48,63,73	1.33	7 (14%)	54,101,113	1.69	10 (18%)
14	CLA	B2	816	-	52,67,73	1.18	7 (13%)	58,105,113	1.53	9 (15%)
14	CLA	B2	817	-	53,68,73	1.29	9 (16%)	60,107,113	1.71	12 (20%)
14	CLA	B2	818	-	58,73,73	1.17	8 (13%)	66,113,113	1.54	8 (12%)
14	CLA	B2	819	-	40,55,73	1.45	7 (17%)	45,91,113	1.75	10 (22%)
14	CLA	B2	820	-	35,53,73	1.45	6 (17%)	38,89,113	1.69	8 (21%)
14	CLA	B2	821	-	48,63,73	1.40	8 (16%)	54,101,113	1.62	9 (16%)
14	CLA	B2	822	-	35,53,73	1.40	7 (20%)	38,89,113	1.71	7 (18%)
14	CLA	B2	823	2	47,62,73	1.37	8 (17%)	52,99,113	1.65	12 (23%)
14	CLA	B2	824	-	39,54,73	1.36	8 (20%)	44,90,113	1.82	10 (22%)
14	CLA	B2	825	-	58,73,73	1.23	7 (12%)	66,113,113	1.62	13 (19%)
14	CLA	B2	826	-	58,73,73	1.19	6 (10%)	66,113,113	1.76	11 (16%)
14	CLA	B2	827	-	58,73,73	1.21	8 (13%)	66,113,113	1.68	11 (16%)
14	CLA	B2	828	-	58,73,73	1.26	8 (13%)	66,113,113	1.75	14 (21%)
14	CLA	B2	829	-	35,53,73	1.38	7 (20%)	38,89,113	1.66	5 (13%)
14	CLA	B2	830	-	42,57,73	1.31	7 (16%)	47,93,113	1.66	10 (21%)
14	CLA	B2	831	-	58,73,73	1.15	8 (13%)	66,113,113	1.47	8 (12%)
14	CLA	B2	832	-	51,66,73	1.38	8 (15%)	57,104,113	1.67	8 (14%)
14	CLA	B2	833	-	35,53,73	1.48	7 (20%)	38,89,113	1.73	7 (18%)
14	CLA	B2	834	-	35,53,73	1.44	7 (20%)	38,89,113	1.80	8 (21%)
14	CLA	B2	835	-	35,53,73	1.48	7 (20%)	38,89,113	1.85	8 (21%)
14	CLA	B2	836	-	53,68,73	1.29	7 (13%)	60,107,113	1.51	8 (13%)
14	CLA	B2	837	-	58,73,73	1.22	8 (13%)	66,113,113	1.41	8 (12%)
14	CLA	B2	838	-	40,55,73	1.25	9 (22%)	45,91,113	1.78	9 (20%)
14	CLA	B2	839	-	58,73,73	1.07	6 (10%)	66,113,113	1.58	9 (13%)
14	CLA	B2	840	-	58,73,73	1.10	6 (10%)	66,113,113	1.59	8 (12%)
15	PQN	B2	841	-	34,34,34	2.13	7 (20%)	42,45,45	1.53	4 (9%)
16	BCR	B2	842	-	41,41,41	1.13	3 (7%)	56,56,56	1.52	10 (17%)
16	BCR	B2	843	-	41,41,41	1.17	3 (7%)	56,56,56	1.63	12 (21%)
16	BCR	B2	844	-	41,41,41	0.91	1 (2%)	56,56,56	1.58	14 (25%)
16	BCR	B2	845	-	25,25,41	0.91	0	33,33,56	1.34	7 (21%)
16	BCR	B2	846	-	41,41,41	0.84	1 (2%)	56,56,56	1.41	11 (19%)
16	BCR	B2	847	-	41,41,41	0.76	0	56,56,56	1.29	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	LMG	B2	848	-	55,55,55	0.85	3 (5%)	63,63,63	1.02	3 (4%)
17	LHG	B2	849	-	22,22,48	1.82	5 (22%)	25,28,54	1.09	1 (4%)
16	BCR	B2	850	-	41,41,41	1.04	2 (4%)	56,56,56	1.38	9 (16%)
14	CLA	B3	1801	17	45,60,73	1.36	8 (17%)	50,97,113	1.78	12 (24%)
14	CLA	B3	1802	-	58,73,73	1.15	6 (10%)	66,113,113	1.64	12 (18%)
14	CLA	B3	1803	-	58,73,73	1.18	9 (15%)	66,113,113	1.67	12 (18%)
14	CLA	B3	1804	-	58,73,73	1.16	9 (15%)	66,113,113	1.83	14 (21%)
14	CLA	B3	1805	-	58,73,73	1.25	9 (15%)	66,113,113	1.37	10 (15%)
14	CLA	B3	1806	-	47,62,73	1.28	6 (12%)	52,99,113	1.78	11 (21%)
14	CLA	B3	1807	-	58,73,73	1.18	7 (12%)	66,113,113	1.63	9 (13%)
14	CLA	B3	1808	-	58,73,73	1.12	8 (13%)	66,113,113	1.50	9 (13%)
14	CLA	B3	1809	-	58,73,73	1.14	8 (13%)	66,113,113	1.52	9 (13%)
14	CLA	B3	1810	-	58,73,73	1.07	6 (10%)	66,113,113	1.74	13 (19%)
14	CLA	B3	1811	2	58,73,73	1.06	7 (12%)	66,113,113	1.76	12 (18%)
14	CLA	B3	1812	2	58,73,73	1.09	6 (10%)	66,113,113	1.71	14 (21%)
14	CLA	B3	1813	-	35,53,73	1.37	7 (20%)	38,89,113	1.83	6 (15%)
14	CLA	B3	1814	-	35,53,73	1.52	6 (17%)	38,89,113	1.75	9 (23%)
14	CLA	B3	1815	-	58,73,73	1.18	7 (12%)	66,113,113	1.64	12 (18%)
14	CLA	B3	1816	-	58,73,73	1.16	7 (12%)	66,113,113	1.60	10 (15%)
14	CLA	B3	1817	-	35,53,73	1.31	5 (14%)	38,89,113	1.96	8 (21%)
14	CLA	B3	1818	-	48,63,73	1.35	7 (14%)	54,101,113	1.74	10 (18%)
14	CLA	B3	1819	-	52,67,73	1.21	8 (15%)	58,105,113	1.61	11 (18%)
14	CLA	B3	1820	-	53,68,73	1.30	8 (15%)	60,107,113	1.73	11 (18%)
14	CLA	B3	1821	-	58,73,73	1.17	7 (12%)	66,113,113	1.48	9 (13%)
14	CLA	B3	1822	-	40,55,73	1.48	7 (17%)	45,91,113	1.73	11 (24%)
14	CLA	B3	1823	-	35,53,73	1.48	6 (17%)	38,89,113	1.73	8 (21%)
14	CLA	B3	1824	-	48,63,73	1.42	7 (14%)	54,101,113	1.62	11 (20%)
14	CLA	B3	1825	-	35,53,73	1.44	7 (20%)	38,89,113	1.75	7 (18%)
14	CLA	B3	1826	-	47,62,73	1.37	9 (19%)	52,99,113	1.64	11 (21%)
14	CLA	B3	1827	-	39,54,73	1.39	8 (20%)	44,90,113	1.84	10 (22%)
14	CLA	B3	1828	-	58,73,73	1.23	7 (12%)	66,113,113	1.62	12 (18%)
14	CLA	B3	1829	-	58,73,73	1.20	7 (12%)	66,113,113	1.71	12 (18%)
14	CLA	B3	1830	-	58,73,73	1.21	7 (12%)	66,113,113	1.64	11 (16%)
14	CLA	B3	1831	-	58,73,73	1.25	8 (13%)	66,113,113	1.70	13 (19%)
14	CLA	B3	1832	-	35,53,73	1.39	6 (17%)	38,89,113	1.71	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B3	1833	-	42,57,73	1.29	7 (16%)	47,93,113	1.64	9 (19%)
14	CLA	B3	1834	-	58,73,73	1.16	8 (13%)	66,113,113	1.49	7 (10%)
14	CLA	B3	1835	-	51,66,73	1.38	7 (13%)	57,104,113	1.65	9 (15%)
14	CLA	B3	1836	-	35,53,73	1.47	7 (20%)	38,89,113	1.74	6 (15%)
14	CLA	B3	1837	-	35,53,73	1.41	7 (20%)	38,89,113	1.76	8 (21%)
14	CLA	B3	1838	-	35,53,73	1.48	7 (20%)	38,89,113	1.81	8 (21%)
14	CLA	B3	1839	-	53,68,73	1.27	8 (15%)	60,107,113	1.54	8 (13%)
14	CLA	B3	1840	-	58,73,73	1.21	8 (13%)	66,113,113	1.42	8 (12%)
14	CLA	B3	1841	-	40,55,73	1.24	7 (17%)	45,91,113	1.83	10 (22%)
14	CLA	B3	1842	-	58,73,73	1.09	6 (10%)	66,113,113	1.57	10 (15%)
14	CLA	B3	1843	-	58,73,73	1.11	6 (10%)	66,113,113	1.55	7 (10%)
15	PQN	B3	1844	-	34,34,34	2.15	8 (23%)	42,45,45	1.50	4 (9%)
16	BCR	B3	1845	-	41,41,41	1.15	3 (7%)	56,56,56	1.49	9 (16%)
16	BCR	B3	1846	-	41,41,41	1.19	4 (9%)	56,56,56	1.65	12 (21%)
16	BCR	B3	1847	-	41,41,41	0.91	1 (2%)	56,56,56	1.60	14 (25%)
16	BCR	B3	1848	-	25,25,41	0.94	0	33,33,56	1.33	6 (18%)
16	BCR	B3	1849	-	41,41,41	0.82	0	56,56,56	1.41	11 (19%)
19	LMG	B3	1850	-	55,55,55	0.86	3 (5%)	63,63,63	1.00	2 (3%)
16	BCR	B3	1851	-	41,41,41	1.05	3 (7%)	56,56,56	1.40	9 (16%)
14	CLA	B4	801	-	58,73,73	1.13	8 (13%)	66,113,113	1.64	12 (18%)
14	CLA	B4	802	-	58,73,73	1.17	6 (10%)	66,113,113	1.62	13 (19%)
14	CLA	B4	803	-	58,73,73	1.20	9 (15%)	66,113,113	1.67	13 (19%)
14	CLA	B4	804	-	58,73,73	1.18	9 (15%)	66,113,113	1.84	13 (19%)
14	CLA	B4	805	-	58,73,73	1.22	9 (15%)	66,113,113	1.36	10 (15%)
14	CLA	B4	806	-	47,62,73	1.27	6 (12%)	52,99,113	1.83	13 (25%)
14	CLA	B4	807	-	58,73,73	1.20	7 (12%)	66,113,113	1.67	11 (16%)
14	CLA	B4	808	-	58,73,73	1.12	8 (13%)	66,113,113	1.54	9 (13%)
14	CLA	B4	809	-	58,73,73	1.13	8 (13%)	66,113,113	1.52	9 (13%)
14	CLA	B4	810	-	58,73,73	1.05	5 (8%)	66,113,113	1.73	12 (18%)
14	CLA	B4	811	2	58,73,73	1.08	7 (12%)	66,113,113	1.76	13 (19%)
14	CLA	B4	812	2	58,73,73	1.10	6 (10%)	66,113,113	1.64	13 (19%)
14	CLA	B4	813	-	35,53,73	1.39	7 (20%)	38,89,113	1.78	6 (15%)
14	CLA	B4	814	-	35,53,73	1.54	6 (17%)	38,89,113	1.73	9 (23%)
14	CLA	B4	815	-	58,73,73	1.18	6 (10%)	66,113,113	1.65	13 (19%)
14	CLA	B4	816	-	58,73,73	1.15	7 (12%)	66,113,113	1.57	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B4	817	-	35,53,73	1.33	5 (14%)	38,89,113	1.94	8 (21%)
14	CLA	B4	818	-	48,63,73	1.33	7 (14%)	54,101,113	1.71	10 (18%)
14	CLA	B4	819	-	52,67,73	1.21	7 (13%)	58,105,113	1.57	11 (18%)
14	CLA	B4	820	-	53,68,73	1.30	8 (15%)	60,107,113	1.68	11 (18%)
14	CLA	B4	821	-	58,73,73	1.19	8 (13%)	66,113,113	1.54	10 (15%)
14	CLA	B4	822	-	40,55,73	1.46	7 (17%)	45,91,113	1.73	10 (22%)
14	CLA	B4	823	-	35,53,73	1.48	6 (17%)	38,89,113	1.68	8 (21%)
14	CLA	B4	824	-	48,63,73	1.45	8 (16%)	54,101,113	1.59	9 (16%)
14	CLA	B4	825	-	35,53,73	1.40	7 (20%)	38,89,113	1.72	7 (18%)
14	CLA	B4	826	2	47,62,73	1.42	9 (19%)	52,99,113	1.62	10 (19%)
14	CLA	B4	827	-	39,54,73	1.40	9 (23%)	44,90,113	1.84	10 (22%)
14	CLA	B4	828	-	58,73,73	1.20	6 (10%)	66,113,113	1.58	13 (19%)
14	CLA	B4	829	-	58,73,73	1.20	7 (12%)	66,113,113	1.69	11 (16%)
14	CLA	B4	830	-	58,73,73	1.20	7 (12%)	66,113,113	1.66	12 (18%)
14	CLA	B4	831	-	58,73,73	1.26	8 (13%)	66,113,113	1.74	15 (22%)
14	CLA	B4	832	-	35,53,73	1.39	7 (20%)	38,89,113	1.68	6 (15%)
14	CLA	B4	833	-	42,57,73	1.31	7 (16%)	47,93,113	1.69	9 (19%)
14	CLA	B4	834	-	58,73,73	1.18	8 (13%)	66,113,113	1.49	9 (13%)
14	CLA	B4	835	-	51,66,73	1.40	8 (15%)	57,104,113	1.65	9 (15%)
14	CLA	B4	836	-	35,53,73	1.49	7 (20%)	38,89,113	1.72	6 (15%)
14	CLA	B4	837	-	35,53,73	1.44	8 (22%)	38,89,113	1.81	9 (23%)
14	CLA	B4	838	-	35,53,73	1.46	7 (20%)	38,89,113	1.83	7 (18%)
14	CLA	B4	839	-	53,68,73	1.28	7 (13%)	60,107,113	1.53	8 (13%)
14	CLA	B4	840	-	58,73,73	1.22	8 (13%)	66,113,113	1.44	10 (15%)
14	CLA	B4	841	-	40,55,73	1.25	7 (17%)	45,91,113	1.79	12 (26%)
14	CLA	B4	842	-	58,73,73	1.08	6 (10%)	66,113,113	1.63	11 (16%)
14	CLA	B4	843	-	58,73,73	1.11	6 (10%)	66,113,113	1.54	8 (12%)
15	PQN	B4	844	-	34,34,34	2.13	7 (20%)	42,45,45	1.52	4 (9%)
16	BCR	B4	845	-	41,41,41	1.15	3 (7%)	56,56,56	1.52	10 (17%)
16	BCR	B4	846	-	41,41,41	1.18	4 (9%)	56,56,56	1.65	14 (25%)
16	BCR	B4	847	-	41,41,41	0.94	1 (2%)	56,56,56	1.57	13 (23%)
16	BCR	B4	848	-	25,25,41	0.92	0	33,33,56	1.33	6 (18%)
16	BCR	B4	849	-	41,41,41	0.86	1 (2%)	56,56,56	1.43	11 (19%)
16	BCR	B4	850	-	41,41,41	0.75	0	56,56,56	1.29	8 (14%)
19	LMG	B4	851	-	55,55,55	0.85	3 (5%)	63,63,63	1.03	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B4	852	17	45,60,73	1.36	8 (17%)	50,97,113	1.74	11 (22%)
14	CLA	B5	1801	17	45,60,73	1.37	8 (17%)	50,97,113	1.78	11 (22%)
14	CLA	B5	1802	-	58,73,73	1.14	6 (10%)	66,113,113	1.62	13 (19%)
14	CLA	B5	1803	-	58,73,73	1.18	9 (15%)	66,113,113	1.63	13 (19%)
14	CLA	B5	1804	-	58,73,73	1.17	9 (15%)	66,113,113	1.83	13 (19%)
14	CLA	B5	1805	-	58,73,73	1.23	9 (15%)	66,113,113	1.42	11 (16%)
14	CLA	B5	1806	-	47,62,73	1.28	6 (12%)	52,99,113	1.79	10 (19%)
14	CLA	B5	1807	-	58,73,73	1.18	7 (12%)	66,113,113	1.66	10 (15%)
14	CLA	B5	1808	-	58,73,73	1.11	8 (13%)	66,113,113	1.53	11 (16%)
14	CLA	B5	1809	-	58,73,73	1.12	8 (13%)	66,113,113	1.53	8 (12%)
14	CLA	B5	1810	-	58,73,73	1.04	5 (8%)	66,113,113	1.71	11 (16%)
14	CLA	B5	1811	2	58,73,73	1.06	7 (12%)	66,113,113	1.76	14 (21%)
14	CLA	B5	1812	2	58,73,73	1.09	6 (10%)	66,113,113	1.65	13 (19%)
14	CLA	B5	1813	-	35,53,73	1.37	7 (20%)	38,89,113	1.76	6 (15%)
14	CLA	B5	1814	-	35,53,73	1.52	6 (17%)	38,89,113	1.72	8 (21%)
14	CLA	B5	1815	-	58,73,73	1.17	6 (10%)	66,113,113	1.55	9 (13%)
14	CLA	B5	1816	-	58,73,73	1.19	7 (12%)	66,113,113	1.62	9 (13%)
14	CLA	B5	1817	-	35,53,73	1.35	6 (17%)	38,89,113	1.91	8 (21%)
14	CLA	B5	1818	-	48,63,73	1.35	6 (12%)	54,101,113	1.72	10 (18%)
14	CLA	B5	1819	-	52,67,73	1.19	7 (13%)	58,105,113	1.59	11 (18%)
14	CLA	B5	1820	-	53,68,73	1.30	8 (15%)	60,107,113	1.71	12 (20%)
14	CLA	B5	1821	-	58,73,73	1.18	8 (13%)	66,113,113	1.60	9 (13%)
14	CLA	B5	1822	-	40,55,73	1.48	7 (17%)	45,91,113	1.77	11 (24%)
14	CLA	B5	1823	-	35,53,73	1.49	6 (17%)	38,89,113	1.73	8 (21%)
14	CLA	B5	1824	-	48,63,73	1.47	7 (14%)	54,101,113	1.63	11 (20%)
14	CLA	B5	1825	-	35,53,73	1.40	6 (17%)	38,89,113	1.71	6 (15%)
14	CLA	B5	1826	-	47,62,73	1.40	9 (19%)	52,99,113	1.64	11 (21%)
14	CLA	B5	1827	-	39,54,73	1.43	9 (23%)	44,90,113	1.83	9 (20%)
14	CLA	B5	1828	-	58,73,73	1.20	6 (10%)	66,113,113	1.57	15 (22%)
14	CLA	B5	1829	-	58,73,73	1.19	7 (12%)	66,113,113	1.72	13 (19%)
14	CLA	B5	1830	-	58,73,73	1.21	7 (12%)	66,113,113	1.64	10 (15%)
14	CLA	B5	1831	-	58,73,73	1.26	8 (13%)	66,113,113	1.66	11 (16%)
14	CLA	B5	1832	-	35,53,73	1.38	7 (20%)	38,89,113	1.65	5 (13%)
14	CLA	B5	1833	-	42,57,73	1.29	7 (16%)	47,93,113	1.64	9 (19%)
14	CLA	B5	1834	-	58,73,73	1.16	8 (13%)	66,113,113	1.53	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B5	1835	-	51,66,73	1.36	7 (13%)	57,104,113	1.65	9 (15%)
14	CLA	B5	1836	-	35,53,73	1.47	7 (20%)	38,89,113	1.70	5 (13%)
14	CLA	B5	1837	-	35,53,73	1.45	8 (22%)	38,89,113	1.78	9 (23%)
14	CLA	B5	1838	-	35,53,73	1.46	7 (20%)	38,89,113	1.78	8 (21%)
14	CLA	B5	1839	-	53,68,73	1.27	8 (15%)	60,107,113	1.50	7 (11%)
14	CLA	B5	1840	-	58,73,73	1.22	8 (13%)	66,113,113	1.44	11 (16%)
14	CLA	B5	1841	-	40,55,73	1.24	7 (17%)	45,91,113	1.81	10 (22%)
14	CLA	B5	1842	-	58,73,73	1.07	6 (10%)	66,113,113	1.60	10 (15%)
14	CLA	B5	1843	-	58,73,73	1.11	6 (10%)	66,113,113	1.59	8 (12%)
15	PQN	B5	1844	-	34,34,34	2.12	7 (20%)	42,45,45	1.53	4 (9%)
16	BCR	B5	1845	-	41,41,41	1.14	3 (7%)	56,56,56	1.49	10 (17%)
16	BCR	B5	1846	-	41,41,41	1.18	3 (7%)	56,56,56	1.66	13 (23%)
16	BCR	B5	1847	-	41,41,41	0.92	1 (2%)	56,56,56	1.58	13 (23%)
16	BCR	B5	1848	-	25,25,41	0.92	0	33,33,56	1.36	6 (18%)
16	BCR	B5	1849	-	41,41,41	0.86	1 (2%)	56,56,56	1.43	13 (23%)
16	BCR	B5	1850	-	41,41,41	0.76	1 (2%)	56,56,56	1.56	12 (21%)
19	LMG	B5	1851	-	55,55,55	0.84	3 (5%)	63,63,63	1.01	2 (3%)
18	SF4	B6	801	2	0,12,12	0.00	-	0,24,24	0.00	-
14	CLA	B6	802	-	58,73,73	1.13	8 (13%)	66,113,113	1.62	12 (18%)
14	CLA	B6	803	-	58,73,73	1.16	8 (13%)	66,113,113	1.38	7 (10%)
14	CLA	B6	804	-	58,73,73	1.19	9 (15%)	66,113,113	1.60	12 (18%)
14	CLA	B6	805	-	58,73,73	1.23	9 (15%)	66,113,113	1.39	10 (15%)
14	CLA	B6	806	-	58,73,73	1.21	7 (12%)	66,113,113	1.64	10 (15%)
14	CLA	B6	807	-	58,73,73	1.12	7 (12%)	66,113,113	1.50	9 (13%)
14	CLA	B6	808	-	58,73,73	1.08	6 (10%)	66,113,113	1.70	11 (16%)
14	CLA	B6	809	-	58,73,73	1.06	6 (10%)	66,113,113	1.73	12 (18%)
14	CLA	B6	810	2	58,73,73	1.08	6 (10%)	66,113,113	1.69	13 (19%)
14	CLA	B6	811	-	35,53,73	1.36	7 (20%)	38,89,113	1.78	6 (15%)
14	CLA	B6	812	-	35,53,73	1.52	6 (17%)	38,89,113	1.73	10 (26%)
14	CLA	B6	813	-	58,73,73	1.18	6 (10%)	66,113,113	1.61	10 (15%)
14	CLA	B6	814	-	58,73,73	1.19	7 (12%)	66,113,113	1.60	8 (12%)
14	CLA	B6	815	-	35,53,73	1.34	5 (14%)	38,89,113	1.93	8 (21%)
14	CLA	B6	816	-	48,63,73	1.33	6 (12%)	54,101,113	1.71	10 (18%)
14	CLA	B6	817	-	52,67,73	1.18	7 (13%)	58,105,113	1.52	11 (18%)
14	CLA	B6	818	-	53,68,73	1.29	8 (15%)	60,107,113	1.73	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B6	819	-	58,73,73	1.17	8 (13%)	66,113,113	1.50	8 (12%)
14	CLA	B6	820	-	40,55,73	1.46	7 (17%)	45,91,113	1.76	10 (22%)
14	CLA	B6	821	-	35,53,73	1.48	6 (17%)	38,89,113	1.71	8 (21%)
14	CLA	B6	822	-	48,63,73	1.43	7 (14%)	54,101,113	1.65	12 (22%)
14	CLA	B6	823	-	35,53,73	1.44	7 (20%)	38,89,113	1.72	6 (15%)
14	CLA	B6	824	2	47,62,73	1.37	9 (19%)	52,99,113	1.67	12 (23%)
14	CLA	B6	825	-	39,54,73	1.37	8 (20%)	44,90,113	1.84	8 (18%)
14	CLA	B6	826	-	58,73,73	1.23	8 (13%)	66,113,113	1.60	13 (19%)
14	CLA	B6	827	-	58,73,73	1.21	7 (12%)	66,113,113	1.71	11 (16%)
14	CLA	B6	828	-	58,73,73	1.21	7 (12%)	66,113,113	1.65	11 (16%)
14	CLA	B6	829	-	58,73,73	1.26	8 (13%)	66,113,113	1.76	15 (22%)
14	CLA	B6	830	-	35,53,73	1.39	7 (20%)	38,89,113	1.70	5 (13%)
14	CLA	B6	831	-	42,57,73	1.30	7 (16%)	47,93,113	1.61	9 (19%)
14	CLA	B6	832	-	58,73,73	1.16	8 (13%)	66,113,113	1.48	8 (12%)
14	CLA	B6	833	-	51,66,73	1.36	7 (13%)	57,104,113	1.69	10 (17%)
14	CLA	B6	834	-	35,53,73	1.47	7 (20%)	38,89,113	1.75	8 (21%)
14	CLA	B6	835	-	35,53,73	1.45	8 (22%)	38,89,113	1.81	8 (21%)
14	CLA	B6	836	-	35,53,73	1.47	7 (20%)	38,89,113	1.81	7 (18%)
14	CLA	B6	837	-	53,68,73	1.28	7 (13%)	60,107,113	1.50	9 (15%)
14	CLA	B6	838	-	58,73,73	1.22	8 (13%)	66,113,113	1.45	12 (18%)
14	CLA	B6	839	-	40,55,73	1.23	7 (17%)	45,91,113	1.85	9 (20%)
14	CLA	B6	840	-	58,73,73	1.09	6 (10%)	66,113,113	1.59	10 (15%)
14	CLA	B6	841	-	58,73,73	1.09	6 (10%)	66,113,113	1.58	9 (13%)
15	PQN	B6	842	-	34,34,34	2.14	7 (20%)	42,45,45	1.52	4 (9%)
16	BCR	B6	843	-	41,41,41	1.14	3 (7%)	56,56,56	1.50	9 (16%)
16	BCR	B6	844	-	41,41,41	1.18	4 (9%)	56,56,56	1.64	14 (25%)
16	BCR	B6	845	-	41,41,41	0.91	2 (4%)	56,56,56	1.59	14 (25%)
16	BCR	B6	846	-	25,25,41	0.92	0	33,33,56	1.33	6 (18%)
16	BCR	B6	847	-	41,41,41	0.85	1 (2%)	56,56,56	1.42	11 (19%)
19	LMG	B6	848	-	55,55,55	0.86	3 (5%)	63,63,63	1.01	3 (4%)
17	LHG	B6	849	-	22,22,48	1.66	5 (22%)	25,28,54	1.07	1 (4%)
16	BCR	B6	850	-	41,41,41	1.04	2 (4%)	56,56,56	1.40	9 (16%)
18	SF4	C1	101	3	0,12,12	0.00	-	0,24,24	0.00	-
18	SF4	C1	102	3	0,12,12	0.00	-	0,24,24	0.00	-
18	SF4	C2	101	3	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	SF4	C2	102	3	0,12,12	0.00	-	0,24,24	0.00	-
18	SF4	C3	101	-	0,12,12	0.00	-	0,24,24	0.00	-
18	SF4	C3	102	3	0,12,12	0.00	-	0,24,24	0.00	-
18	SF4	C4	101	3	0,12,12	0.00	-	0,24,24	0.00	-
18	SF4	C4	102	3	0,12,12	0.00	-	0,24,24	0.00	-
18	SF4	C5	101	3	0,12,12	0.00	-	0,24,24	0.00	-
18	SF4	C5	102	3	0,12,12	0.00	-	0,24,24	0.00	-
18	SF4	C6	101	3	0,12,12	0.00	-	0,24,24	0.00	-
18	SF4	C6	102	3	0,12,12	0.00	-	0,24,24	0.00	-
14	CLA	F1	1301	-	35,53,73	1.46	6 (17%)	38,89,113	1.87	7 (18%)
16	BCR	F1	1302	-	41,41,41	0.87	1 (2%)	56,56,56	1.38	11 (19%)
16	BCR	F2	201	-	41,41,41	0.75	0	56,56,56	1.54	11 (19%)
14	CLA	F2	202	-	35,53,73	1.47	6 (17%)	38,89,113	1.81	7 (18%)
16	BCR	F2	203	-	41,41,41	0.87	0	56,56,56	1.38	10 (17%)
14	CLA	F2	204	-	31,45,73	1.58	6 (19%)	34,78,113	1.67	7 (20%)
16	BCR	F3	201	-	41,41,41	0.74	1 (2%)	56,56,56	1.55	11 (19%)
14	CLA	F3	202	-	35,53,73	1.46	6 (17%)	38,89,113	1.88	7 (18%)
16	BCR	F3	203	-	41,41,41	0.86	1 (2%)	56,56,56	1.39	10 (17%)
16	BCR	F4	201	-	41,41,41	0.78	0	56,56,56	1.56	11 (19%)
14	CLA	F4	202	-	35,53,73	1.49	6 (17%)	38,89,113	1.81	7 (18%)
16	BCR	F4	203	-	41,41,41	0.90	1 (2%)	56,56,56	1.38	10 (17%)
16	BCR	F4	204	-	41,41,41	1.05	3 (7%)	56,56,56	1.40	9 (16%)
14	CLA	F5	1301	-	35,53,73	1.47	5 (14%)	38,89,113	1.82	7 (18%)
16	BCR	F5	1302	-	41,41,41	0.83	0	56,56,56	1.39	11 (19%)
16	BCR	F6	201	-	41,41,41	0.74	0	56,56,56	1.54	12 (21%)
14	CLA	F6	202	-	35,53,73	1.46	5 (14%)	38,89,113	1.87	7 (18%)
16	BCR	F6	203	-	41,41,41	0.86	0	56,56,56	1.38	10 (17%)
14	CLA	I1	101	-	58,73,73	1.08	7 (12%)	66,113,113	1.60	10 (15%)
16	BCR	I1	102	-	41,41,41	0.72	0	56,56,56	1.39	8 (14%)
16	BCR	I1	103	-	41,41,41	0.85	1 (2%)	56,56,56	1.46	12 (21%)
16	BCR	I2	101	-	41,41,41	0.69	0	56,56,56	1.36	7 (12%)
16	BCR	I3	101	-	41,41,41	0.71	0	56,56,56	1.38	9 (16%)
16	BCR	I3	102	-	41,41,41	0.71	0	56,56,56	1.44	11 (19%)
16	BCR	I4	101	-	41,41,41	0.70	0	56,56,56	1.38	8 (14%)
16	BCR	I4	102	-	41,41,41	0.70	0	56,56,56	1.43	12 (21%)
16	BCR	I5	101	-	41,41,41	0.73	0	56,56,56	1.39	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	I5	102	-	41,41,41	0.74	0	56,56,56	1.42	12 (21%)
14	CLA	I6	101	-	58,73,73	1.08	8 (13%)	66,113,113	1.50	7 (10%)
16	BCR	I6	102	-	41,41,41	0.70	0	56,56,56	1.39	8 (14%)
14	CLA	J1	101	8	35,53,73	1.57	7 (20%)	38,89,113	1.70	7 (18%)
14	CLA	J1	102	-	31,45,73	1.60	6 (19%)	34,78,113	1.65	6 (17%)
16	BCR	J1	103	-	41,41,41	0.85	1 (2%)	56,56,56	1.56	14 (25%)
16	BCR	J1	104	-	41,41,41	0.92	2 (4%)	56,56,56	1.47	11 (19%)
14	CLA	J2	101	8	35,53,73	1.54	7 (20%)	38,89,113	1.75	10 (26%)
16	BCR	J2	102	-	41,41,41	0.82	1 (2%)	56,56,56	1.55	14 (25%)
16	BCR	J2	103	-	41,41,41	0.88	2 (4%)	56,56,56	1.46	10 (17%)
14	CLA	J3	101	8	35,53,73	1.53	7 (20%)	38,89,113	1.75	9 (23%)
14	CLA	J3	102	-	31,45,73	1.62	6 (19%)	34,78,113	1.72	7 (20%)
16	BCR	J3	103	-	41,41,41	0.82	0	56,56,56	1.56	14 (25%)
16	BCR	J3	104	-	41,41,41	0.86	1 (2%)	56,56,56	1.47	12 (21%)
14	CLA	J4	101	8	35,53,73	1.54	7 (20%)	38,89,113	1.79	10 (26%)
14	CLA	J4	102	-	31,45,73	1.58	6 (19%)	34,78,113	1.68	7 (20%)
16	BCR	J4	103	-	41,41,41	0.86	2 (4%)	56,56,56	1.55	14 (25%)
16	BCR	J4	104	-	41,41,41	0.91	2 (4%)	56,56,56	1.45	11 (19%)
14	CLA	J5	101	8	35,53,73	1.53	7 (20%)	38,89,113	1.73	7 (18%)
14	CLA	J5	102	-	31,45,73	1.58	6 (19%)	34,78,113	1.62	7 (20%)
16	BCR	J5	103	-	41,41,41	0.81	0	56,56,56	1.57	14 (25%)
16	BCR	J5	104	-	41,41,41	0.90	1 (2%)	56,56,56	1.47	12 (21%)
16	BCR	J5	105	-	41,41,41	1.06	3 (7%)	56,56,56	1.39	8 (14%)
14	CLA	J6	1101	-	58,73,73	1.10	7 (12%)	66,113,113	1.50	10 (15%)
14	CLA	J6	1102	8	35,53,73	1.51	7 (20%)	38,89,113	1.74	9 (23%)
14	CLA	J6	1103	-	31,45,73	1.58	6 (19%)	34,78,113	1.70	7 (20%)
16	BCR	J6	1104	-	41,41,41	0.80	0	56,56,56	1.56	14 (25%)
16	BCR	J6	1105	-	41,41,41	0.85	1 (2%)	56,56,56	1.45	12 (21%)
14	CLA	K1	1401	-	35,53,73	1.43	7 (20%)	38,89,113	1.89	8 (21%)
14	CLA	K2	1401	-	35,53,73	1.41	7 (20%)	38,89,113	1.90	8 (21%)
14	CLA	K3	1401	-	35,53,73	1.41	7 (20%)	38,89,113	1.89	8 (21%)
14	CLA	K4	1401	-	35,53,73	1.44	7 (20%)	38,89,113	1.89	9 (23%)
14	CLA	K5	101	-	32,49,73	1.44	5 (15%)	34,83,113	1.69	5 (14%)
14	CLA	K5	102	-	35,53,73	1.41	7 (20%)	38,89,113	1.90	9 (23%)
14	CLA	K6	1401	-	35,53,73	1.42	7 (20%)	38,89,113	1.86	9 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	L1	201	-	58,73,73	1.26	9 (15%)	66,113,113	1.61	12 (18%)
14	CLA	L1	202	-	58,73,73	1.09	8 (13%)	66,113,113	1.64	11 (16%)
16	BCR	L1	203	-	41,41,41	0.74	0	56,56,56	1.42	11 (19%)
14	CLA	L1	205	10	58,73,73	1.13	6 (10%)	66,113,113	1.55	9 (13%)
14	CLA	L1	206	-	58,73,73	1.15	7 (12%)	66,113,113	1.46	8 (12%)
14	CLA	L1	207	-	58,73,73	1.18	8 (13%)	66,113,113	1.58	8 (12%)
16	BCR	L1	209	-	41,41,41	1.05	2 (4%)	56,56,56	1.31	7 (12%)
16	BCR	L2	201	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	7 (12%)
14	CLA	L2	202	-	58,73,73	1.09	7 (12%)	66,113,113	1.61	11 (16%)
16	BCR	L2	203	-	41,41,41	0.71	0	56,56,56	1.42	12 (21%)
14	CLA	L2	205	10	58,73,73	1.14	6 (10%)	66,113,113	1.58	10 (15%)
14	CLA	L2	206	-	58,73,73	1.13	7 (12%)	66,113,113	1.48	11 (16%)
14	CLA	L2	207	-	58,73,73	1.17	8 (13%)	66,113,113	1.59	7 (10%)
16	BCR	L2	208	-	41,41,41	0.84	1 (2%)	56,56,56	1.46	11 (19%)
16	BCR	L3	201	-	41,41,41	1.01	2 (4%)	56,56,56	1.25	7 (12%)
14	CLA	L3	202	-	35,53,73	1.53	7 (20%)	38,89,113	1.89	9 (23%)
14	CLA	L3	203	-	58,73,73	1.13	7 (12%)	66,113,113	1.55	11 (16%)
14	CLA	L3	204	-	58,73,73	1.14	7 (12%)	66,113,113	1.48	8 (12%)
14	CLA	L3	205	-	58,73,73	1.17	8 (13%)	66,113,113	1.61	7 (10%)
16	BCR	L3	206	-	41,41,41	0.84	1 (2%)	56,56,56	1.46	12 (21%)
14	CLA	L4	201	-	58,73,73	1.07	7 (12%)	66,113,113	1.65	11 (16%)
14	CLA	L4	203	-	58,73,73	1.14	6 (10%)	66,113,113	1.55	10 (15%)
14	CLA	L4	204	-	58,73,73	1.13	7 (12%)	66,113,113	1.47	9 (13%)
14	CLA	L4	205	-	58,73,73	1.17	7 (12%)	66,113,113	1.61	7 (10%)
16	BCR	L4	206	-	41,41,41	0.84	1 (2%)	56,56,56	1.46	12 (21%)
16	BCR	L4	208	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	7 (12%)
16	BCR	L5	201	-	41,41,41	1.02	2 (4%)	56,56,56	1.27	7 (12%)
14	CLA	L5	202	-	35,53,73	1.55	7 (20%)	38,89,113	1.91	9 (23%)
14	CLA	L5	203	-	58,73,73	1.08	7 (12%)	66,113,113	1.66	10 (15%)
14	CLA	L5	204	10	58,73,73	1.14	6 (10%)	66,113,113	1.54	9 (13%)
14	CLA	L5	205	-	58,73,73	1.15	7 (12%)	66,113,113	1.43	6 (9%)
14	CLA	L5	206	-	58,73,73	1.18	8 (13%)	66,113,113	1.58	8 (12%)
16	BCR	L5	207	-	41,41,41	0.83	1 (2%)	56,56,56	1.47	12 (21%)
16	BCR	L6	201	-	41,41,41	1.02	2 (4%)	56,56,56	1.28	6 (10%)
14	CLA	L6	202	-	58,73,73	1.23	7 (12%)	66,113,113	1.63	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	L6	203	-	58,73,73	1.09	8 (13%)	66,113,113	1.67	13 (19%)
16	BCR	L6	204	-	41,41,41	0.74	0	56,56,56	1.43	13 (23%)
14	CLA	L6	206	10	58,73,73	1.14	6 (10%)	66,113,113	1.56	10 (15%)
14	CLA	L6	207	-	58,73,73	1.14	7 (12%)	66,113,113	1.46	10 (15%)
14	CLA	L6	208	-	58,73,73	1.17	8 (13%)	66,113,113	1.62	9 (13%)
16	BCR	L6	209	-	41,41,41	0.84	1 (2%)	56,56,56	1.44	11 (19%)
14	CLA	M1	1201	-	47,62,73	1.30	6 (12%)	52,99,113	1.82	13 (25%)
16	BCR	M1	1202	-	41,41,41	0.87	1 (2%)	56,56,56	1.46	10 (17%)
14	CLA	M2	1201	-	47,62,73	1.27	5 (10%)	52,99,113	1.84	13 (25%)
16	BCR	M2	1202	-	41,41,41	0.85	1 (2%)	56,56,56	1.45	10 (17%)
14	CLA	M3	1601	-	35,53,73	1.53	7 (20%)	38,89,113	1.88	9 (23%)
16	BCR	M3	1602	-	41,41,41	0.84	1 (2%)	56,56,56	1.46	12 (21%)
16	BCR	M4	101	-	41,41,41	0.82	0	56,56,56	1.46	13 (23%)
16	BCR	M5	101	-	41,41,41	0.85	1 (2%)	56,56,56	1.47	12 (21%)
14	CLA	M6	1201	-	47,62,73	1.27	6 (12%)	52,99,113	1.79	12 (23%)
16	BCR	M6	1202	-	41,41,41	0.84	1 (2%)	56,56,56	1.47	11 (19%)
21	FES	P1	101	13	0,4,4	0.00	-	0,4,4	0.00	-
21	FES	P2	101	13	0,4,4	0.00	-	0,4,4	0.00	-
21	FES	P3	101	13	0,4,4	0.00	-	0,4,4	0.00	-
21	FES	P4	101	13	0,4,4	0.00	-	0,4,4	0.00	-
21	FES	P5	101	13	0,4,4	0.00	-	0,4,4	0.00	-
21	FES	P6	101	13	0,4,4	0.00	-	0,4,4	0.00	-
14	CLA	X1	1701	-	35,53,73	1.54	7 (20%)	38,89,113	1.77	7 (18%)
14	CLA	X2	1701	12	35,53,73	1.55	7 (20%)	38,89,113	1.75	9 (23%)
17	LHG	X3	101	-	22,22,48	1.84	5 (22%)	25,28,54	1.08	1 (4%)
14	CLA	X3	102	12	35,53,73	1.55	7 (20%)	38,89,113	1.73	7 (18%)
17	LHG	X4	101	-	22,22,48	1.67	5 (22%)	25,28,54	1.07	1 (4%)
14	CLA	X4	102	12	35,53,73	1.59	7 (20%)	38,89,113	1.75	8 (21%)
14	CLA	X5	101	12	35,53,73	1.53	7 (20%)	38,89,113	1.79	7 (18%)
17	LHG	X5	102	-	22,22,48	1.64	5 (22%)	25,28,54	1.09	1 (4%)
14	CLA	X6	1701	-	35,53,73	1.57	7 (20%)	38,89,113	1.76	7 (18%)

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
14	CLA	A1	801	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	802	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	803	14	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A1	804	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	805	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	806	-	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A1	807	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	808	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	809	-	1/1/16/25	0/11/111/135	0/0/9/9
14	CLA	A1	810	14	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	811	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A1	812	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	A1	813	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A1	814	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A1	815	-	2/2/16/25	1/18/116/135	0/0/9/9
14	CLA	A1	816	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A1	817	-	1/1/17/25	0/24/122/135	0/0/9/9
14	CLA	A1	818	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	819	-	2/2/19/25	0/33/131/135	0/0/9/9
14	CLA	A1	820	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	821	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	A1	822	-	1/1/17/25	0/21/119/135	0/0/9/9
14	CLA	A1	823	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A1	824	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	825	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	826	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	827	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	828	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	829	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	830	-	2/2/17/25	0/19/117/135	0/0/9/9
14	CLA	A1	831	-	-	0/37/135/135	0/0/9/9
14	CLA	A1	832	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A1	833	1	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A1	834	-	3/3/17/25	0/21/119/135	0/0/9/9
14	CLA	A1	835	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	836	-	1/1/16/25	0/16/114/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A1	837	-	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A1	838	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	839	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A1	840	-	3/3/14/25	0/5/101/135	0/0/9/9
15	PQN	A1	841	-	-	0/23/43/43	0/2/2/2
16	BCR	A1	842	-	-	0/29/63/63	0/2/2/2
16	BCR	A1	843	-	-	0/29/63/63	0/2/2/2
16	BCR	A1	844	-	-	0/29/63/63	0/2/2/2
16	BCR	A1	845	-	-	0/29/63/63	0/2/2/2
16	BCR	A1	846	-	-	0/29/63/63	0/2/2/2
16	BCR	A1	847	-	-	0/29/63/63	0/2/2/2
17	LHG	A1	848	-	-	0/53/53/53	0/0/0/0
17	LHG	A1	849	14	1/1/5/5	0/31/31/53	0/0/0/0
18	SF4	A1	850	-	-	0/0/48/48	0/6/5/5
14	CLA	A2	1601	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A2	1602	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1603	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1604	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1605	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1606	14	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A2	1607	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1608	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1609	-	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A2	1610	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1611	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1612	-	1/1/16/25	0/11/111/135	0/0/9/9
14	CLA	A2	1613	14	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1614	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A2	1615	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	A2	1616	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A2	1617	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A2	1618	-	2/2/16/25	1/18/116/135	0/0/9/9
14	CLA	A2	1619	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A2	1620	-	1/1/17/25	0/24/122/135	0/0/9/9
14	CLA	A2	1621	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1622	-	2/2/19/25	0/33/131/135	0/0/9/9
14	CLA	A2	1623	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A2	1624	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	A2	1625	-	1/1/17/25	0/21/119/135	0/0/9/9
14	CLA	A2	1626	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A2	1627	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1628	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1629	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1630	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1631	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1632	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1633	-	2/2/17/25	0/19/117/135	0/0/9/9
14	CLA	A2	1634	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1635	-	-	0/37/135/135	0/0/9/9
14	CLA	A2	1636	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A2	1637	1	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A2	1638	-	3/3/17/25	0/21/119/135	0/0/9/9
14	CLA	A2	1639	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1640	-	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	A2	1641	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1642	-	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A2	1643	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1644	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A2	1645	-	3/3/14/25	0/5/101/135	0/0/9/9
15	PQN	A2	1646	-	-	0/23/43/43	0/2/2/2
16	BCR	A2	1647	-	-	0/29/63/63	0/2/2/2
16	BCR	A2	1648	-	-	0/29/63/63	0/2/2/2
16	BCR	A2	1649	-	-	0/29/63/63	0/2/2/2
16	BCR	A2	1650	-	-	0/29/63/63	0/2/2/2
16	BCR	A2	1651	-	-	0/29/63/63	0/2/2/2
16	BCR	A2	1652	-	-	0/29/63/63	0/2/2/2
17	LHG	A2	1653	-	-	0/53/53/53	0/0/0/0
17	LHG	A2	1654	14	1/1/5/5	0/31/31/53	0/0/0/0
18	SF4	A2	1655	1,2	-	0/0/48/48	0/6/5/5
14	CLA	A3	801	-	-	0/37/135/135	0/0/9/9
14	CLA	A3	802	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	803	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	804	14	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A3	805	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A3	806	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	807	-	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A3	808	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	809	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	810	-	1/1/16/25	0/11/111/135	0/0/9/9
14	CLA	A3	811	14	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	812	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A3	813	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	A3	814	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A3	815	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A3	816	-	2/2/16/25	1/18/116/135	0/0/9/9
14	CLA	A3	817	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A3	818	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A3	819	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	820	-	2/2/19/25	0/33/131/135	0/0/9/9
14	CLA	A3	821	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	822	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	A3	823	-	1/1/17/25	0/21/119/135	0/0/9/9
14	CLA	A3	824	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A3	825	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	826	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	827	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	828	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	829	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	830	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	831	-	2/2/17/25	0/19/117/135	0/0/9/9
14	CLA	A3	832	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	833	-	-	0/37/135/135	0/0/9/9
14	CLA	A3	834	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	835	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A3	836	1	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A3	837	-	3/3/17/25	0/21/119/135	0/0/9/9
14	CLA	A3	838	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	839	-	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	A3	840	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A3	841	-	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A3	842	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	843	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A3	844	-	3/3/14/25	0/5/101/135	0/0/9/9
14	CLA	A3	845	17	2/2/17/25	0/22/120/135	0/0/9/9
15	PQN	A3	846	-	-	0/23/43/43	0/2/2/2
16	BCR	A3	847	-	-	0/29/63/63	0/2/2/2
16	BCR	A3	848	-	-	0/29/63/63	0/2/2/2
16	BCR	A3	849	-	-	0/29/63/63	0/2/2/2
16	BCR	A3	850	-	-	0/29/63/63	0/2/2/2
16	BCR	A3	851	-	-	0/29/63/63	0/2/2/2
16	BCR	A3	852	-	-	0/29/63/63	0/2/2/2
17	LHG	A3	853	-	-	0/53/53/53	0/0/0/0
17	LHG	A3	854	14	1/1/5/5	0/31/31/53	0/0/0/0
18	SF4	A3	855	-	-	0/0/48/48	0/6/5/5
16	BCR	A3	856	-	-	0/29/63/63	0/2/2/2
14	CLA	A4	801	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	802	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	803	14	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A4	804	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	805	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	806	-	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A4	807	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	808	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	809	-	1/1/16/25	0/11/111/135	0/0/9/9
14	CLA	A4	810	14	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	811	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A4	812	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	A4	813	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A4	814	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A4	815	-	2/2/16/25	1/18/116/135	0/0/9/9
14	CLA	A4	816	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A4	817	-	1/1/17/25	0/24/122/135	0/0/9/9
14	CLA	A4	818	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	819	-	2/2/19/25	0/33/131/135	0/0/9/9
14	CLA	A4	820	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	821	-	2/2/16/25	0/18/116/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A4	822	-	1/1/17/25	0/21/119/135	0/0/9/9
14	CLA	A4	823	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A4	824	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	825	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	826	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	827	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	828	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	829	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	830	-	2/2/17/25	0/19/117/135	0/0/9/9
14	CLA	A4	831	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	832	-	-	0/37/135/135	0/0/9/9
14	CLA	A4	833	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A4	834	1	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A4	835	-	3/3/17/25	0/21/119/135	0/0/9/9
14	CLA	A4	836	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	837	-	-	0/16/114/135	0/0/9/9
14	CLA	A4	838	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	839	-	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A4	840	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	841	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A4	842	-	3/3/14/25	0/5/101/135	0/0/9/9
15	PQN	A4	843	-	-	0/23/43/43	0/2/2/2
16	BCR	A4	844	-	-	0/29/63/63	0/2/2/2
16	BCR	A4	845	-	-	0/29/63/63	0/2/2/2
16	BCR	A4	846	-	-	0/29/63/63	0/2/2/2
16	BCR	A4	847	-	-	0/29/63/63	0/2/2/2
16	BCR	A4	848	-	-	0/29/63/63	0/2/2/2
16	BCR	A4	849	-	-	0/29/63/63	0/2/2/2
17	LHG	A4	850	-	-	0/53/53/53	0/0/0/0
17	LHG	A4	851	14	1/1/5/5	0/31/31/53	0/0/0/0
18	SF4	A4	852	1,2	-	0/0/48/48	0/6/5/5
14	CLA	A4	853	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A5	801	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	802	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	803	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	804	14	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A5	805	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A5	806	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	807	-	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A5	808	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	809	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	810	-	1/1/16/25	0/11/111/135	0/0/9/9
14	CLA	A5	811	14	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	812	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A5	813	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	A5	814	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A5	815	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A5	816	-	2/2/16/25	1/18/116/135	0/0/9/9
14	CLA	A5	817	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A5	818	-	1/1/17/25	0/24/122/135	0/0/9/9
14	CLA	A5	819	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	820	-	2/2/19/25	0/33/131/135	0/0/9/9
14	CLA	A5	821	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	822	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	A5	823	-	1/1/17/25	0/21/119/135	0/0/9/9
14	CLA	A5	824	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A5	825	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	826	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	827	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	828	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	829	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	830	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	831	-	2/2/17/25	0/19/117/135	0/0/9/9
14	CLA	A5	832	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	833	-	-	0/37/135/135	0/0/9/9
14	CLA	A5	834	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A5	835	1	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A5	836	-	3/3/17/25	0/21/119/135	0/0/9/9
14	CLA	A5	837	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	838	-	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	A5	839	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	840	-	2/2/17/25	0/21/119/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A5	841	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	842	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A5	843	17	2/2/17/25	0/22/120/135	0/0/9/9
15	PQN	A5	844	-	-	0/23/43/43	0/2/2/2
16	BCR	A5	845	-	-	0/29/63/63	0/2/2/2
16	BCR	A5	846	-	-	0/29/63/63	0/2/2/2
16	BCR	A5	847	-	-	0/29/63/63	0/2/2/2
16	BCR	A5	848	-	-	0/29/63/63	0/2/2/2
16	BCR	A5	849	-	-	0/29/63/63	0/2/2/2
16	BCR	A5	850	-	-	0/29/63/63	0/2/2/2
17	LHG	A5	851	-	-	0/53/53/53	0/0/0/0
17	LHG	A5	852	14	1/1/5/5	0/31/31/53	0/0/0/0
16	BCR	A5	853	-	-	0/29/63/63	0/2/2/2
18	SF4	A5	854	1	-	0/0/48/48	0/6/5/5
14	CLA	A6	1601	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A6	1602	-	-	0/37/135/135	0/0/9/9
14	CLA	A6	1603	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1604	14	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A6	1605	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1606	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1607	-	1/1/17/25	0/21/119/135	0/0/9/9
14	CLA	A6	1608	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1609	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1610	-	1/1/16/25	0/11/111/135	0/0/9/9
14	CLA	A6	1611	14	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1612	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A6	1613	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	A6	1614	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A6	1615	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A6	1616	-	2/2/16/25	1/18/116/135	0/0/9/9
14	CLA	A6	1617	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A6	1618	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A6	1619	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1620	-	2/2/19/25	0/33/131/135	0/0/9/9
14	CLA	A6	1621	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1622	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	A6	1623	-	1/1/17/25	0/21/119/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A6	1624	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	A6	1625	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1626	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1627	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1628	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1629	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1630	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1631	-	2/2/17/25	0/19/117/135	0/0/9/9
14	CLA	A6	1632	-	-	0/37/135/135	0/0/9/9
14	CLA	A6	1633	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1634	-	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	A6	1635	1	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	A6	1636	-	3/3/17/25	0/21/119/135	0/0/9/9
14	CLA	A6	1637	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1638	-	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	A6	1639	-	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A6	1640	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A6	1641	-	3/3/14/25	0/5/101/135	0/0/9/9
15	PQN	A6	1642	-	-	0/23/43/43	0/2/2/2
16	BCR	A6	1643	-	-	0/29/63/63	0/2/2/2
16	BCR	A6	1644	-	-	0/29/63/63	0/2/2/2
16	BCR	A6	1645	-	-	0/29/63/63	0/2/2/2
16	BCR	A6	1646	-	-	0/29/63/63	0/2/2/2
16	BCR	A6	1647	-	-	0/29/63/63	0/2/2/2
16	BCR	A6	1648	-	-	0/29/63/63	0/2/2/2
17	LHG	A6	1649	-	-	0/53/53/53	0/0/0/0
17	LHG	A6	1650	14	1/1/5/5	0/31/31/53	0/0/0/0
14	CLA	A6	1651	-	1/1/20/25	0/37/135/135	0/0/9/9
16	BCR	A6	1652	-	-	0/29/63/63	0/2/2/2
14	CLA	B1	801	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	802	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	803	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	804	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	805	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	806	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	807	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	808	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	809	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B1	810	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	811	-	-	0/37/135/135	0/0/9/9
14	CLA	B1	812	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B1	813	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B1	814	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	815	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	816	-	1/1/16/25	0/11/111/135	0/0/9/9
14	CLA	B1	817	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B1	818	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	B1	819	-	1/1/19/25	0/31/129/135	0/0/9/9
14	CLA	B1	820	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	821	-	2/2/16/25	0/16/114/135	0/0/9/9
14	CLA	B1	822	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B1	823	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B1	824	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B1	825	-	3/3/17/25	0/24/122/135	0/0/9/9
14	CLA	B1	826	-	2/2/16/25	0/15/113/135	0/0/9/9
14	CLA	B1	827	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	828	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	829	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	830	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	831	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B1	832	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	B1	833	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	834	-	2/2/18/25	0/29/127/135	0/0/9/9
14	CLA	B1	835	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B1	836	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B1	837	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B1	838	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	B1	839	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B1	840	-	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	B1	841	-	2/2/20/25	0/37/135/135	0/0/9/9
15	PQN	B1	842	-	-	0/23/43/43	0/2/2/2
16	BCR	B1	843	-	-	0/29/63/63	0/2/2/2
16	BCR	B1	844	-	-	0/29/63/63	0/2/2/2
16	BCR	B1	845	-	-	0/29/63/63	0/2/2/2
16	BCR	B1	846	-	-	0/18/35/63	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	B1	847	-	-	0/29/63/63	0/2/2/2
16	BCR	B1	848	-	-	0/29/63/63	0/2/2/2
16	BCR	B1	849	-	-	0/29/63/63	0/2/2/2
19	LMG	B1	850	-	-	0/50/70/70	0/1/1/1
17	LHG	B1	851	-	-	0/26/26/53	0/0/0/0
16	BCR	B1	852	-	-	0/29/63/63	0/2/2/2
14	CLA	B1	853	17	2/2/17/25	0/22/120/135	0/0/9/9
14	CLA	B1	854	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	801	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	802	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	803	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	804	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	805	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	806	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	807	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	808	2	-	0/37/135/135	0/0/9/9
14	CLA	B2	809	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	810	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B2	811	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B2	812	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	813	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	814	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B2	815	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B2	816	-	1/1/18/25	0/30/128/135	0/0/9/9
14	CLA	B2	817	-	2/2/19/25	0/31/129/135	0/0/9/9
14	CLA	B2	818	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	819	-	2/2/16/25	0/16/114/135	0/0/9/9
14	CLA	B2	820	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B2	821	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B2	822	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B2	823	2	3/3/17/25	0/24/122/135	0/0/9/9
14	CLA	B2	824	-	2/2/16/25	0/15/113/135	0/0/9/9
14	CLA	B2	825	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	826	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	827	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	828	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	829	-	2/2/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B2	830	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	B2	831	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	832	-	2/2/18/25	0/29/127/135	0/0/9/9
14	CLA	B2	833	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B2	834	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B2	835	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B2	836	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	B2	837	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	838	-	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	B2	839	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B2	840	-	2/2/20/25	0/37/135/135	0/0/9/9
15	PQN	B2	841	-	-	0/23/43/43	0/2/2/2
16	BCR	B2	842	-	-	0/29/63/63	0/2/2/2
16	BCR	B2	843	-	-	0/29/63/63	0/2/2/2
16	BCR	B2	844	-	-	0/29/63/63	0/2/2/2
16	BCR	B2	845	-	-	0/18/35/63	0/1/1/2
16	BCR	B2	846	-	-	0/29/63/63	0/2/2/2
16	BCR	B2	847	-	-	0/29/63/63	0/2/2/2
19	LMG	B2	848	-	-	0/50/70/70	0/1/1/1
17	LHG	B2	849	-	-	0/26/26/53	0/0/0/0
16	BCR	B2	850	-	-	0/29/63/63	0/2/2/2
14	CLA	B3	1801	17	2/2/17/25	0/22/120/135	0/0/9/9
14	CLA	B3	1802	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1803	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1804	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1805	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1806	-	1/1/17/25	0/24/122/135	0/0/9/9
14	CLA	B3	1807	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1808	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1809	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1810	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1811	2	-	0/37/135/135	0/0/9/9
14	CLA	B3	1812	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1813	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B3	1814	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B3	1815	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1816	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1817	-	1/1/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B3	1818	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B3	1819	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	B3	1820	-	1/1/19/25	0/31/129/135	0/0/9/9
14	CLA	B3	1821	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1822	-	2/2/16/25	0/16/114/135	0/0/9/9
14	CLA	B3	1823	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B3	1824	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B3	1825	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B3	1826	-	3/3/17/25	0/24/122/135	0/0/9/9
14	CLA	B3	1827	-	2/2/16/25	0/15/113/135	0/0/9/9
14	CLA	B3	1828	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1829	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1830	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1831	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1832	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B3	1833	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	B3	1834	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1835	-	2/2/18/25	0/29/127/135	0/0/9/9
14	CLA	B3	1836	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B3	1837	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B3	1838	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B3	1839	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	B3	1840	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1841	-	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	B3	1842	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B3	1843	-	2/2/20/25	0/37/135/135	0/0/9/9
15	PQN	B3	1844	-	-	0/23/43/43	0/2/2/2
16	BCR	B3	1845	-	-	0/29/63/63	0/2/2/2
16	BCR	B3	1846	-	-	0/29/63/63	0/2/2/2
16	BCR	B3	1847	-	-	0/29/63/63	0/2/2/2
16	BCR	B3	1848	-	-	0/18/35/63	0/1/1/2
16	BCR	B3	1849	-	-	0/29/63/63	0/2/2/2
19	LMG	B3	1850	-	-	0/50/70/70	0/1/1/1
16	BCR	B3	1851	-	-	0/29/63/63	0/2/2/2
14	CLA	B4	801	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	802	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	803	-	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B4	804	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	805	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	806	-	1/1/17/25	0/24/122/135	0/0/9/9
14	CLA	B4	807	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	808	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	809	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	810	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	811	2	-	0/37/135/135	0/0/9/9
14	CLA	B4	812	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	813	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B4	814	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B4	815	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	816	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	817	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B4	818	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B4	819	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	B4	820	-	1/1/19/25	0/31/129/135	0/0/9/9
14	CLA	B4	821	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	822	-	2/2/16/25	0/16/114/135	0/0/9/9
14	CLA	B4	823	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B4	824	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B4	825	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B4	826	2	3/3/17/25	0/24/122/135	0/0/9/9
14	CLA	B4	827	-	2/2/16/25	0/15/113/135	0/0/9/9
14	CLA	B4	828	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	829	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	830	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	831	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	832	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B4	833	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	B4	834	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	835	-	2/2/18/25	0/29/127/135	0/0/9/9
14	CLA	B4	836	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B4	837	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B4	838	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B4	839	-	3/3/19/25	0/31/129/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B4	840	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	841	-	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	B4	842	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B4	843	-	2/2/20/25	0/37/135/135	0/0/9/9
15	PQN	B4	844	-	-	0/23/43/43	0/2/2/2
16	BCR	B4	845	-	-	0/29/63/63	0/2/2/2
16	BCR	B4	846	-	-	0/29/63/63	0/2/2/2
16	BCR	B4	847	-	-	0/29/63/63	0/2/2/2
16	BCR	B4	848	-	-	0/18/35/63	0/1/1/2
16	BCR	B4	849	-	-	0/29/63/63	0/2/2/2
16	BCR	B4	850	-	-	0/29/63/63	0/2/2/2
19	LMG	B4	851	-	-	0/50/70/70	0/1/1/1
14	CLA	B4	852	17	2/2/17/25	0/22/120/135	0/0/9/9
14	CLA	B5	1801	17	2/2/17/25	0/22/120/135	0/0/9/9
14	CLA	B5	1802	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1803	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1804	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1805	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1806	-	1/1/17/25	0/24/122/135	0/0/9/9
14	CLA	B5	1807	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1808	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1809	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1810	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1811	2	-	0/37/135/135	0/0/9/9
14	CLA	B5	1812	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1813	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B5	1814	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B5	1815	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1816	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1817	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B5	1818	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B5	1819	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	B5	1820	-	2/2/19/25	0/31/129/135	0/0/9/9
14	CLA	B5	1821	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1822	-	2/2/16/25	0/16/114/135	0/0/9/9
14	CLA	B5	1823	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B5	1824	-	2/2/18/25	0/25/123/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B5	1825	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B5	1826	-	3/3/17/25	0/24/122/135	0/0/9/9
14	CLA	B5	1827	-	2/2/16/25	0/15/113/135	0/0/9/9
14	CLA	B5	1828	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1829	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1830	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1831	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1832	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B5	1833	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	B5	1834	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1835	-	2/2/18/25	0/29/127/135	0/0/9/9
14	CLA	B5	1836	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B5	1837	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B5	1838	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B5	1839	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	B5	1840	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1841	-	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	B5	1842	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B5	1843	-	2/2/20/25	0/37/135/135	0/0/9/9
15	PQN	B5	1844	-	-	0/23/43/43	0/2/2/2
16	BCR	B5	1845	-	-	0/29/63/63	0/2/2/2
16	BCR	B5	1846	-	-	0/29/63/63	0/2/2/2
16	BCR	B5	1847	-	-	0/29/63/63	0/2/2/2
16	BCR	B5	1848	-	-	0/18/35/63	0/1/1/2
16	BCR	B5	1849	-	-	0/29/63/63	0/2/2/2
16	BCR	B5	1850	-	-	0/29/63/63	0/2/2/2
19	LMG	B5	1851	-	-	0/50/70/70	0/1/1/1
18	SF4	B6	801	2	-	0/0/48/48	0/6/5/5
14	CLA	B6	802	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	803	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	804	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	805	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	806	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	807	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	808	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	809	-	-	0/37/135/135	0/0/9/9
14	CLA	B6	810	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	811	-	2/2/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B6	812	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B6	813	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	814	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	815	-	1/1/16/25	0/11/111/135	0/0/9/9
14	CLA	B6	816	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B6	817	-	2/2/18/25	0/30/128/135	0/0/9/9
14	CLA	B6	818	-	2/2/19/25	0/31/129/135	0/0/9/9
14	CLA	B6	819	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	820	-	2/2/16/25	0/16/114/135	0/0/9/9
14	CLA	B6	821	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B6	822	-	2/2/18/25	0/25/123/135	0/0/9/9
14	CLA	B6	823	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B6	824	2	3/3/17/25	0/24/122/135	0/0/9/9
14	CLA	B6	825	-	2/2/16/25	0/15/113/135	0/0/9/9
14	CLA	B6	826	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	827	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	828	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	829	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	830	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B6	831	-	2/2/16/25	0/18/116/135	0/0/9/9
14	CLA	B6	832	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	833	-	2/2/18/25	0/29/127/135	0/0/9/9
14	CLA	B6	834	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B6	835	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B6	836	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B6	837	-	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	B6	838	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	839	-	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	B6	840	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B6	841	-	2/2/20/25	0/37/135/135	0/0/9/9
15	PQN	B6	842	-	-	0/23/43/43	0/2/2/2
16	BCR	B6	843	-	-	0/29/63/63	0/2/2/2
16	BCR	B6	844	-	-	0/29/63/63	0/2/2/2
16	BCR	B6	845	-	-	0/29/63/63	0/2/2/2
16	BCR	B6	846	-	-	0/18/35/63	0/1/1/2
16	BCR	B6	847	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LMG	B6	848	-	-	0/50/70/70	0/1/1/1
17	LHG	B6	849	-	-	0/26/26/53	0/0/0/0
16	BCR	B6	850	-	-	0/29/63/63	0/2/2/2
18	SF4	C1	101	3	-	0/0/48/48	0/6/5/5
18	SF4	C1	102	3	-	0/0/48/48	0/6/5/5
18	SF4	C2	101	3	-	0/0/48/48	0/6/5/5
18	SF4	C2	102	3	-	0/0/48/48	0/6/5/5
18	SF4	C3	101	-	-	0/0/48/48	0/6/5/5
18	SF4	C3	102	3	-	0/0/48/48	0/6/5/5
18	SF4	C4	101	3	-	0/0/48/48	0/6/5/5
18	SF4	C4	102	3	-	0/0/48/48	0/6/5/5
18	SF4	C5	101	3	-	0/0/48/48	0/6/5/5
18	SF4	C5	102	3	-	0/0/48/48	0/6/5/5
18	SF4	C6	101	3	-	0/0/48/48	0/6/5/5
18	SF4	C6	102	3	-	0/0/48/48	0/6/5/5
14	CLA	F1	1301	-	2/2/16/25	0/11/111/135	0/0/9/9
16	BCR	F1	1302	-	-	0/29/63/63	0/2/2/2
16	BCR	F2	201	-	-	0/29/63/63	0/2/2/2
14	CLA	F2	202	-	2/2/16/25	0/11/111/135	0/0/9/9
16	BCR	F2	203	-	-	0/29/63/63	0/2/2/2
14	CLA	F2	204	-	2/2/13/25	0/2/96/135	0/0/9/9
16	BCR	F3	201	-	-	0/29/63/63	0/2/2/2
14	CLA	F3	202	-	2/2/16/25	0/11/111/135	0/0/9/9
16	BCR	F3	203	-	-	0/29/63/63	0/2/2/2
16	BCR	F4	201	-	-	0/29/63/63	0/2/2/2
14	CLA	F4	202	-	2/2/16/25	0/11/111/135	0/0/9/9
16	BCR	F4	203	-	-	0/29/63/63	0/2/2/2
16	BCR	F4	204	-	-	0/29/63/63	0/2/2/2
14	CLA	F5	1301	-	2/2/16/25	0/11/111/135	0/0/9/9
16	BCR	F5	1302	-	-	0/29/63/63	0/2/2/2
16	BCR	F6	201	-	-	0/29/63/63	0/2/2/2
14	CLA	F6	202	-	2/2/16/25	0/11/111/135	0/0/9/9
16	BCR	F6	203	-	-	0/29/63/63	0/2/2/2
14	CLA	I1	101	-	2/2/20/25	0/37/135/135	0/0/9/9
16	BCR	I1	102	-	-	0/29/63/63	0/2/2/2
16	BCR	I1	103	-	-	0/29/63/63	0/2/2/2
16	BCR	I2	101	-	-	0/29/63/63	0/2/2/2
16	BCR	I3	101	-	-	0/29/63/63	0/2/2/2
16	BCR	I3	102	-	-	0/29/63/63	0/2/2/2
16	BCR	I4	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	I4	102	-	-	0/29/63/63	0/2/2/2
16	BCR	I5	101	-	-	0/29/63/63	0/2/2/2
16	BCR	I5	102	-	-	0/29/63/63	0/2/2/2
14	CLA	I6	101	-	1/1/20/25	0/37/135/135	0/0/9/9
16	BCR	I6	102	-	-	0/29/63/63	0/2/2/2
14	CLA	J1	101	8	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	J1	102	-	2/2/13/25	0/2/96/135	0/0/9/9
16	BCR	J1	103	-	-	0/29/63/63	0/2/2/2
16	BCR	J1	104	-	-	0/29/63/63	0/2/2/2
14	CLA	J2	101	8	3/3/16/25	0/11/111/135	0/0/9/9
16	BCR	J2	102	-	-	0/29/63/63	0/2/2/2
16	BCR	J2	103	-	-	0/29/63/63	0/2/2/2
14	CLA	J3	101	8	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	J3	102	-	2/2/13/25	0/2/96/135	0/0/9/9
16	BCR	J3	103	-	-	0/29/63/63	0/2/2/2
16	BCR	J3	104	-	-	0/29/63/63	0/2/2/2
14	CLA	J4	101	8	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	J4	102	-	2/2/13/25	0/2/96/135	0/0/9/9
16	BCR	J4	103	-	-	0/29/63/63	0/2/2/2
16	BCR	J4	104	-	-	0/29/63/63	0/2/2/2
14	CLA	J5	101	8	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	J5	102	-	2/2/13/25	0/2/96/135	0/0/9/9
16	BCR	J5	103	-	-	0/29/63/63	0/2/2/2
16	BCR	J5	104	-	-	0/29/63/63	0/2/2/2
16	BCR	J5	105	-	-	0/29/63/63	0/2/2/2
14	CLA	J6	1101	-	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	J6	1102	8	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	J6	1103	-	2/2/13/25	0/2/96/135	0/0/9/9
16	BCR	J6	1104	-	-	0/29/63/63	0/2/2/2
16	BCR	J6	1105	-	-	0/29/63/63	0/2/2/2
14	CLA	K1	1401	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	K2	1401	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	K3	1401	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	K4	1401	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	K5	101	-	3/3/14/25	0/5/101/135	0/0/9/9
14	CLA	K5	102	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	K6	1401	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	L1	201	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	L1	202	-	2/2/20/25	0/37/135/135	0/0/9/9
16	BCR	L1	203	-	-	0/29/63/63	0/2/2/2
14	CLA	L1	205	10	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	L1	206	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L1	207	-	1/1/20/25	0/37/135/135	0/0/9/9
16	BCR	L1	209	-	-	0/29/63/63	0/2/2/2
16	BCR	L2	201	-	-	0/29/63/63	0/2/2/2
14	CLA	L2	202	-	2/2/20/25	0/37/135/135	0/0/9/9
16	BCR	L2	203	-	-	0/29/63/63	0/2/2/2
14	CLA	L2	205	10	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	L2	206	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L2	207	-	2/2/20/25	0/37/135/135	0/0/9/9
16	BCR	L2	208	-	-	0/29/63/63	0/2/2/2
16	BCR	L3	201	-	-	0/29/63/63	0/2/2/2
14	CLA	L3	202	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	L3	203	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L3	204	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L3	205	-	1/1/20/25	0/37/135/135	0/0/9/9
16	BCR	L3	206	-	-	0/29/63/63	0/2/2/2
14	CLA	L4	201	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L4	203	-	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	L4	204	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L4	205	-	2/2/20/25	0/37/135/135	0/0/9/9
16	BCR	L4	206	-	-	0/29/63/63	0/2/2/2
16	BCR	L4	208	-	-	0/29/63/63	0/2/2/2
16	BCR	L5	201	-	-	0/29/63/63	0/2/2/2
14	CLA	L5	202	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	L5	203	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L5	204	10	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L5	205	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L5	206	-	1/1/20/25	0/37/135/135	0/0/9/9
16	BCR	L5	207	-	-	0/29/63/63	0/2/2/2
16	BCR	L6	201	-	-	0/29/63/63	0/2/2/2
14	CLA	L6	202	-	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L6	203	-	2/2/20/25	0/37/135/135	0/0/9/9
16	BCR	L6	204	-	-	0/29/63/63	0/2/2/2
14	CLA	L6	206	10	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L6	207	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	L6	208	-	1/1/20/25	0/37/135/135	0/0/9/9
16	BCR	L6	209	-	-	0/29/63/63	0/2/2/2
14	CLA	M1	1201	-	1/1/17/25	0/24/122/135	0/0/9/9
16	BCR	M1	1202	-	-	0/29/63/63	0/2/2/2
14	CLA	M2	1201	-	1/1/17/25	0/24/122/135	0/0/9/9
16	BCR	M2	1202	-	-	0/29/63/63	0/2/2/2
14	CLA	M3	1601	-	2/2/16/25	0/11/111/135	0/0/9/9
16	BCR	M3	1602	-	-	0/29/63/63	0/2/2/2
16	BCR	M4	101	-	-	0/29/63/63	0/2/2/2
16	BCR	M5	101	-	-	0/29/63/63	0/2/2/2
14	CLA	M6	1201	-	1/1/17/25	0/24/122/135	0/0/9/9
16	BCR	M6	1202	-	-	0/29/63/63	0/2/2/2
21	FES	P1	101	13	-	0/0/4/4	0/1/1/1
21	FES	P2	101	13	-	0/0/4/4	0/1/1/1
21	FES	P3	101	13	-	0/0/4/4	0/1/1/1
21	FES	P4	101	13	-	0/0/4/4	0/1/1/1
21	FES	P5	101	13	-	0/0/4/4	0/1/1/1
21	FES	P6	101	13	-	0/0/4/4	0/1/1/1
14	CLA	X1	1701	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	X2	1701	12	2/2/16/25	0/11/111/135	0/0/9/9
17	LHG	X3	101	-	-	0/26/26/53	0/0/0/0
14	CLA	X3	102	12	2/2/16/25	0/11/111/135	0/0/9/9
17	LHG	X4	101	-	-	0/26/26/53	0/0/0/0
14	CLA	X4	102	12	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	X5	101	12	2/2/16/25	0/11/111/135	0/0/9/9
17	LHG	X5	102	-	-	0/26/26/53	0/0/0/0
14	CLA	X6	1701	-	2/2/16/25	0/11/111/135	0/0/9/9

All (4397) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A5	844	PQN	C2M-C2	-3.60	1.43	1.50
15	A1	841	PQN	C2M-C2	-3.59	1.43	1.50
15	A6	1642	PQN	C2M-C2	-3.57	1.43	1.50
15	A2	1646	PQN	C2M-C2	-3.53	1.43	1.50
15	A3	846	PQN	C2M-C2	-3.50	1.43	1.50
15	A4	843	PQN	C2M-C2	-3.50	1.43	1.50
15	B2	841	PQN	C2M-C2	-3.48	1.43	1.50
15	B6	842	PQN	C2M-C2	-3.46	1.43	1.50
15	B3	1844	PQN	C2M-C2	-3.46	1.43	1.50
15	B5	1844	PQN	C2M-C2	-3.45	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B1	842	PQN	C2M-C2	-3.44	1.43	1.50
15	B4	844	PQN	C2M-C2	-3.42	1.43	1.50
14	B6	802	CLA	C4A-NA	-2.71	1.34	1.38
14	B4	801	CLA	C4A-NA	-2.71	1.34	1.38
14	A3	802	CLA	C4A-NA	-2.70	1.34	1.38
14	B1	801	CLA	C4A-NA	-2.64	1.34	1.38
14	A5	802	CLA	C4A-NA	-2.64	1.34	1.38
14	A2	1603	CLA	C4A-NA	-2.63	1.34	1.38
14	B1	819	CLA	C4A-NA	-2.59	1.34	1.38
14	L2	202	CLA	C4A-NA	-2.58	1.34	1.38
14	A6	1633	CLA	C4A-NA	-2.56	1.34	1.38
14	L1	202	CLA	C4A-NA	-2.55	1.34	1.38
14	L5	203	CLA	C4A-NA	-2.55	1.34	1.38
15	B3	1844	PQN	C16-C15	-2.54	1.42	1.52
14	A3	834	CLA	C4A-NA	-2.54	1.34	1.38
14	L4	201	CLA	C4A-NA	-2.53	1.34	1.38
15	B1	842	PQN	C16-C15	-2.53	1.42	1.52
14	B5	1820	CLA	C4A-NA	-2.53	1.34	1.38
14	A6	1651	CLA	C4A-NA	-2.53	1.34	1.38
14	B6	818	CLA	C4A-NA	-2.51	1.34	1.38
14	A3	831	CLA	C4A-NA	-2.49	1.34	1.38
14	B4	820	CLA	C4A-NA	-2.47	1.34	1.38
15	B4	844	PQN	C16-C15	-2.47	1.43	1.52
15	B2	841	PQN	C16-C15	-2.47	1.43	1.52
15	B5	1844	PQN	C16-C15	-2.46	1.43	1.52
15	B6	842	PQN	C16-C15	-2.45	1.43	1.52
14	A5	821	CLA	C4A-NA	-2.45	1.34	1.38
14	B3	1820	CLA	C4A-NA	-2.45	1.34	1.38
14	B2	831	CLA	C4A-NA	-2.45	1.34	1.38
14	B2	817	CLA	C4A-NA	-2.43	1.34	1.38
14	B5	1834	CLA	C4A-NA	-2.43	1.34	1.38
14	B6	832	CLA	C4A-NA	-2.42	1.34	1.38
14	A6	1631	CLA	C4A-NA	-2.42	1.34	1.38
14	B2	823	CLA	C4A-NA	-2.42	1.34	1.38
14	B6	805	CLA	C4A-NA	-2.41	1.34	1.38
14	B1	833	CLA	C4A-NA	-2.41	1.34	1.38
14	B2	802	CLA	C4A-NA	-2.40	1.34	1.38
14	B4	803	CLA	C4A-NA	-2.39	1.34	1.38
14	B3	1813	CLA	C4A-NA	-2.38	1.34	1.38
14	B4	834	CLA	C4A-NA	-2.38	1.34	1.38
14	B3	1809	CLA	C4A-NA	-2.38	1.34	1.38
14	A5	803	CLA	C4A-NA	-2.38	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A3	821	CLA	C4A-NA	-2.37	1.34	1.38
14	B5	1804	CLA	C4A-NA	-2.36	1.34	1.38
14	B3	1804	CLA	C4A-NA	-2.36	1.34	1.38
14	A2	1633	CLA	C4A-NA	-2.36	1.34	1.38
14	A6	1621	CLA	C4A-NA	-2.36	1.34	1.38
14	A1	830	CLA	C4A-NA	-2.35	1.34	1.38
14	A3	820	CLA	C4A-NA	-2.35	1.34	1.38
14	B3	1805	CLA	C4A-NA	-2.35	1.34	1.38
14	B4	809	CLA	C4A-NA	-2.35	1.34	1.38
14	B1	805	CLA	C4A-NA	-2.35	1.34	1.38
14	B5	1805	CLA	C4A-NA	-2.34	1.34	1.38
14	B1	825	CLA	C4A-NA	-2.34	1.34	1.38
15	A6	1642	PQN	C16-C15	-2.34	1.43	1.52
14	A2	1605	CLA	C4A-NA	-2.34	1.34	1.38
14	I6	101	CLA	C4A-NA	-2.34	1.34	1.38
15	A4	843	PQN	C16-C15	-2.33	1.43	1.52
14	B2	810	CLA	C4A-NA	-2.33	1.34	1.38
14	A4	830	CLA	C4A-NA	-2.33	1.34	1.38
14	B4	826	CLA	C4A-NA	-2.33	1.34	1.38
14	B6	824	CLA	C4A-NA	-2.33	1.34	1.38
14	B2	801	CLA	C4A-NA	-2.33	1.34	1.38
15	A5	844	PQN	C16-C15	-2.32	1.43	1.52
14	A5	831	CLA	C4A-NA	-2.32	1.34	1.38
15	A2	1646	PQN	C16-C15	-2.32	1.43	1.52
14	B6	811	CLA	C4A-NA	-2.32	1.34	1.38
15	A3	846	PQN	C16-C15	-2.31	1.43	1.52
15	A1	841	PQN	C16-C15	-2.30	1.43	1.52
14	B1	806	CLA	C4A-NA	-2.30	1.34	1.38
14	A1	802	CLA	C4A-NA	-2.29	1.34	1.38
14	A4	802	CLA	C4A-NA	-2.29	1.34	1.38
14	B6	804	CLA	C4A-NA	-2.29	1.34	1.38
14	A4	820	CLA	C4A-NA	-2.28	1.34	1.38
14	B2	806	CLA	C4A-NA	-2.28	1.34	1.38
14	B2	803	CLA	C4A-NA	-2.28	1.34	1.38
14	B3	1834	CLA	C4A-NA	-2.27	1.34	1.38
14	B1	809	CLA	C4A-NA	-2.27	1.34	1.38
14	B2	829	CLA	C4A-NA	-2.26	1.34	1.38
14	B1	802	CLA	C4A-NA	-2.26	1.34	1.38
14	B4	804	CLA	C4A-NA	-2.25	1.34	1.38
14	B4	802	CLA	C4A-NA	-2.25	1.34	1.38
14	A2	1604	CLA	C4A-NA	-2.24	1.34	1.38
14	A6	1603	CLA	C4A-NA	-2.24	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A3	803	CLA	C4A-NA	-2.23	1.34	1.38
14	B1	840	CLA	C4A-NA	-2.23	1.34	1.38
14	B6	830	CLA	C4A-NA	-2.23	1.34	1.38
14	B5	1803	CLA	C4A-NA	-2.23	1.34	1.38
14	A2	1622	CLA	C4A-NA	-2.23	1.34	1.38
14	J6	1101	CLA	C4A-NA	-2.22	1.34	1.38
14	B4	813	CLA	C4A-NA	-2.22	1.34	1.38
14	A6	1606	CLA	C4A-NA	-2.22	1.34	1.38
14	A4	801	CLA	C4A-NA	-2.22	1.34	1.38
14	A2	1608	CLA	C4A-NA	-2.22	1.34	1.38
14	A3	806	CLA	C4A-NA	-2.21	1.34	1.38
14	B5	1809	CLA	C4A-NA	-2.21	1.34	1.38
14	B4	805	CLA	C4A-NA	-2.20	1.34	1.38
14	B3	1802	CLA	C4A-NA	-2.20	1.34	1.38
14	B5	1802	CLA	C4A-NA	-2.20	1.34	1.38
14	A2	1623	CLA	C4A-NA	-2.20	1.34	1.38
14	B5	1841	CLA	C4A-NA	-2.20	1.34	1.38
14	B5	1813	CLA	C4A-NA	-2.20	1.34	1.38
14	B3	1826	CLA	C4A-NA	-2.19	1.34	1.38
14	A5	827	CLA	C4A-NA	-2.19	1.34	1.38
14	A5	806	CLA	C4A-NA	-2.19	1.34	1.38
14	A3	808	CLA	C4A-NA	-2.19	1.34	1.38
14	A1	819	CLA	C4A-NA	-2.18	1.34	1.38
14	A5	820	CLA	C4A-NA	-2.18	1.34	1.38
14	A1	820	CLA	C4A-NA	-2.18	1.34	1.38
14	B4	836	CLA	C4A-NA	-2.17	1.34	1.38
14	A6	1627	CLA	C4A-NA	-2.17	1.34	1.38
14	B3	1803	CLA	C4A-NA	-2.17	1.34	1.38
14	A4	805	CLA	C4A-NA	-2.17	1.34	1.38
14	A5	801	CLA	C4A-NA	-2.17	1.34	1.38
14	B3	1836	CLA	C4A-NA	-2.16	1.34	1.38
14	B1	804	CLA	C4A-NA	-2.16	1.34	1.38
14	B4	811	CLA	C4A-NA	-2.16	1.34	1.38
14	A3	819	CLA	C4A-NA	-2.16	1.34	1.38
14	A6	1608	CLA	C4A-NA	-2.16	1.34	1.38
14	B6	834	CLA	C4A-NA	-2.15	1.34	1.38
14	B5	1826	CLA	C4A-NA	-2.15	1.34	1.38
14	A6	1620	CLA	C4A-NA	-2.15	1.34	1.38
14	A2	1629	CLA	C4A-NA	-2.15	1.34	1.38
14	B1	808	CLA	C4A-NA	-2.15	1.34	1.38
14	B5	1811	CLA	C4A-NA	-2.15	1.34	1.38
14	A6	1619	CLA	C4A-NA	-2.14	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B4	832	CLA	C4A-NA	-2.14	1.34	1.38
14	A1	805	CLA	C4A-NA	-2.13	1.34	1.38
14	B1	812	CLA	C4A-NA	-2.13	1.34	1.38
14	B5	1837	CLA	C4A-NA	-2.12	1.34	1.38
14	B1	831	CLA	C4A-NA	-2.12	1.34	1.38
14	B6	839	CLA	C4A-NA	-2.12	1.34	1.38
14	A2	1610	CLA	C4A-NA	-2.12	1.34	1.38
14	A6	1622	CLA	C4A-NA	-2.12	1.34	1.38
14	A1	826	CLA	C4A-NA	-2.12	1.34	1.38
14	A4	819	CLA	C4A-NA	-2.12	1.34	1.38
19	B5	1851	LMG	O7-C8	-2.11	1.41	1.46
14	A3	805	CLA	C4A-NA	-2.11	1.35	1.38
14	A5	808	CLA	C4A-NA	-2.11	1.35	1.38
14	B6	825	CLA	C4A-NA	-2.10	1.35	1.38
14	B3	1808	CLA	C4A-NA	-2.10	1.35	1.38
14	A6	1602	CLA	C4A-NA	-2.10	1.35	1.38
14	B3	1832	CLA	C4A-NA	-2.10	1.35	1.38
14	A1	807	CLA	C4A-NA	-2.10	1.35	1.38
14	A1	801	CLA	C4A-NA	-2.10	1.35	1.38
14	A4	807	CLA	C4A-NA	-2.09	1.35	1.38
14	A2	1630	CLA	C4A-NA	-2.09	1.35	1.38
14	A5	819	CLA	C4A-NA	-2.09	1.35	1.38
14	B5	1808	CLA	C4A-NA	-2.08	1.35	1.38
14	B4	808	CLA	C4A-NA	-2.08	1.35	1.38
14	B5	1839	CLA	C4A-NA	-2.08	1.35	1.38
14	A3	822	CLA	C4A-NA	-2.08	1.35	1.38
14	B4	827	CLA	C4A-NA	-2.08	1.35	1.38
19	B1	850	LMG	O7-C8	-2.08	1.41	1.46
14	A6	1614	CLA	C4A-NA	-2.08	1.35	1.38
14	A1	818	CLA	C4A-NA	-2.08	1.35	1.38
14	B6	814	CLA	C4A-NA	-2.07	1.35	1.38
14	B1	811	CLA	C4A-NA	-2.07	1.35	1.38
14	B4	841	CLA	C4A-NA	-2.07	1.35	1.38
14	A3	828	CLA	C4A-NA	-2.07	1.35	1.38
14	B2	838	CLA	C4A-NA	-2.07	1.35	1.38
14	A3	826	CLA	C4A-NA	-2.07	1.35	1.38
14	A3	801	CLA	C4A-NA	-2.07	1.35	1.38
14	B2	805	CLA	C4A-NA	-2.06	1.35	1.38
14	B2	833	CLA	C4A-NA	-2.06	1.35	1.38
14	B3	1839	CLA	C4A-NA	-2.06	1.35	1.38
19	B4	851	LMG	O7-C8	-2.05	1.41	1.46
14	B4	837	CLA	C4A-NA	-2.05	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B1	853	CLA	C4A-NA	-2.05	1.35	1.38
14	B3	1841	CLA	C4A-NA	-2.05	1.35	1.38
14	A3	840	CLA	C4A-NA	-2.04	1.35	1.38
14	A1	825	CLA	C4A-NA	-2.04	1.35	1.38
14	L1	201	CLA	C4A-NA	-2.04	1.35	1.38
19	B2	848	LMG	O7-C8	-2.04	1.41	1.46
14	A2	1637	CLA	C4A-NA	-2.03	1.35	1.38
14	A4	818	CLA	C4A-NA	-2.03	1.35	1.38
14	A6	1618	CLA	C4A-NA	-2.03	1.35	1.38
14	B3	1811	CLA	C4A-NA	-2.03	1.35	1.38
14	A2	1624	CLA	C4A-NA	-2.03	1.35	1.38
14	A2	1628	CLA	C4A-NA	-2.03	1.35	1.38
14	B2	824	CLA	C4A-NA	-2.03	1.35	1.38
14	A3	832	CLA	C4A-NA	-2.03	1.35	1.38
14	A6	1628	CLA	C4A-NA	-2.03	1.35	1.38
14	B2	808	CLA	C4A-NA	-2.03	1.35	1.38
14	B5	1832	CLA	C4A-NA	-2.02	1.35	1.38
14	A6	1605	CLA	C4A-NA	-2.02	1.35	1.38
14	B2	832	CLA	C4A-NA	-2.02	1.35	1.38
14	A5	842	CLA	C4A-NA	-2.02	1.35	1.38
14	B1	836	CLA	C4A-NA	-2.02	1.35	1.38
14	A3	827	CLA	C4A-NA	-2.02	1.35	1.38
19	B3	1850	LMG	O7-C8	-2.02	1.41	1.46
14	A1	827	CLA	C4A-NA	-2.02	1.35	1.38
14	A6	1629	CLA	C4A-NA	-2.02	1.35	1.38
14	A3	818	CLA	C4A-NA	-2.02	1.35	1.38
19	B6	848	LMG	O7-C8	-2.02	1.41	1.46
14	B6	835	CLA	C4A-NA	-2.02	1.35	1.38
14	A5	822	CLA	C4A-NA	-2.02	1.35	1.38
14	B6	803	CLA	C4A-NA	-2.02	1.35	1.38
14	B5	1836	CLA	C4A-NA	-2.01	1.35	1.38
14	B3	1827	CLA	C4A-NA	-2.01	1.35	1.38
14	A6	1626	CLA	C4A-NA	-2.01	1.35	1.38
14	B4	835	CLA	C4A-NA	-2.01	1.35	1.38
14	B5	1827	CLA	C4A-NA	-2.01	1.35	1.38
14	A5	828	CLA	C4A-NA	-2.01	1.35	1.38
14	B3	1819	CLA	C4A-NA	-2.01	1.35	1.38
14	L6	203	CLA	C4A-NA	-2.00	1.35	1.38
14	A4	838	CLA	C4A-NA	-2.00	1.35	1.38
14	A5	839	CLA	C4A-NA	-2.00	1.35	1.38
14	A2	1621	CLA	C4A-NA	-2.00	1.35	1.38
14	J5	102	CLA	C1C-C2C	2.00	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B2	827	CLA	C1C-C2C	2.00	1.48	1.44
14	A5	837	CLA	C3C-C2C	2.00	1.41	1.36
14	B1	824	CLA	C1C-C2C	2.00	1.48	1.44
14	A5	807	CLA	C3D-C2D	2.00	1.43	1.39
14	B6	839	CLA	C1C-C2C	2.00	1.48	1.44
14	A6	1610	CLA	C3D-C2D	2.00	1.43	1.39
16	B5	1850	BCR	C5-C6	2.00	1.37	1.34
14	A3	829	CLA	C3C-C2C	2.00	1.41	1.36
14	B2	821	CLA	C3B-C2B	2.01	1.43	1.40
14	A1	818	CLA	C3B-CAB	2.01	1.51	1.47
14	A5	816	CLA	C3C-C2C	2.01	1.41	1.36
14	B1	840	CLA	C3C-C2C	2.01	1.41	1.36
14	B1	840	CLA	C1C-C2C	2.01	1.48	1.44
14	A2	1621	CLA	C2-C3	2.01	1.37	1.33
14	A5	803	CLA	C3C-C2C	2.01	1.41	1.36
14	A4	831	CLA	C1C-C2C	2.01	1.48	1.44
14	A5	804	CLA	C3D-C2D	2.01	1.43	1.39
14	B5	1816	CLA	C3D-C2D	2.01	1.43	1.39
14	A4	801	CLA	C3C-C2C	2.01	1.41	1.36
14	A4	835	CLA	OBD-CAD	2.01	1.25	1.22
14	B4	805	CLA	C4C-C3C	2.01	1.48	1.45
16	F4	204	BCR	C5-C6	2.01	1.37	1.34
14	L6	203	CLA	C1C-C2C	2.01	1.48	1.44
14	A5	811	CLA	C3C-C2C	2.01	1.41	1.36
14	B2	812	CLA	C1C-C2C	2.01	1.48	1.44
14	A6	1611	CLA	O2A-CGA	2.01	1.39	1.33
14	L6	207	CLA	O2A-CGA	2.01	1.39	1.33
14	A6	1613	CLA	C3C-C2C	2.01	1.41	1.36
14	A1	831	CLA	C3D-C2D	2.01	1.43	1.39
14	A2	1630	CLA	O2A-CGA	2.01	1.39	1.33
16	B1	848	BCR	C5-C6	2.01	1.37	1.34
14	A5	810	CLA	C3D-C2D	2.01	1.43	1.39
16	J4	104	BCR	C30-C25	2.01	1.56	1.53
14	A2	1632	CLA	C1C-C2C	2.01	1.48	1.44
14	L1	201	CLA	C1C-C2C	2.01	1.48	1.44
14	A1	815	CLA	C3C-C2C	2.02	1.41	1.36
14	L1	202	CLA	C3C-C2C	2.02	1.41	1.36
14	B3	1810	CLA	C3D-C2D	2.02	1.43	1.39
14	B6	803	CLA	C3D-C2D	2.02	1.43	1.39
14	B6	808	CLA	CHB-C4A	2.02	1.35	1.33
14	X1	1701	CLA	C1C-C2C	2.02	1.48	1.44
14	A3	827	CLA	C3D-C2D	2.02	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A1	825	CLA	C1C-C2C	2.02	1.48	1.44
14	A6	1651	CLA	C4C-C3C	2.02	1.48	1.45
14	B4	821	CLA	C1C-C2C	2.02	1.48	1.44
16	B1	845	BCR	C5-C6	2.02	1.37	1.34
14	A6	1624	CLA	C3D-C2D	2.02	1.43	1.39
16	F3	203	BCR	C30-C25	2.02	1.56	1.53
14	A1	826	CLA	O2D-CGD	2.02	1.38	1.33
14	A4	807	CLA	C3D-C2D	2.02	1.43	1.39
14	B5	1835	CLA	C3D-C2D	2.02	1.43	1.39
14	A1	835	CLA	C3C-C2C	2.02	1.41	1.36
14	B1	841	CLA	C3D-C2D	2.02	1.43	1.39
14	B2	813	CLA	C3D-C2D	2.02	1.43	1.39
14	A3	811	CLA	C3C-C2C	2.02	1.41	1.36
14	B1	825	CLA	C5-C3	2.02	1.55	1.51
16	A5	849	BCR	C1-C6	2.02	1.56	1.53
14	B2	838	CLA	C1C-C2C	2.02	1.48	1.44
14	A2	1605	CLA	C3C-C2C	2.02	1.41	1.36
14	A6	1611	CLA	C3C-C2C	2.02	1.41	1.36
14	L3	203	CLA	C3C-C2C	2.02	1.41	1.36
16	J4	103	BCR	C1-C6	2.02	1.56	1.53
14	A1	817	CLA	C1C-C2C	2.03	1.48	1.44
14	B2	822	CLA	C1C-C2C	2.03	1.48	1.44
14	F2	202	CLA	C3C-C2C	2.03	1.41	1.36
14	A4	810	CLA	O2A-CGA	2.03	1.39	1.33
16	B1	845	BCR	C30-C25	2.03	1.56	1.53
14	A5	813	CLA	C3C-C2C	2.03	1.41	1.36
14	A6	1630	CLA	C1C-C2C	2.03	1.48	1.44
14	B4	816	CLA	C3D-C2D	2.03	1.43	1.39
14	A1	826	CLA	OBD-CAD	2.03	1.25	1.22
14	B2	828	CLA	C3C-C2C	2.03	1.41	1.36
14	A1	813	CLA	C1C-C2C	2.03	1.48	1.44
16	M6	1202	BCR	C1-C6	2.03	1.56	1.53
14	A1	833	CLA	C1C-C2C	2.03	1.48	1.44
14	A1	826	CLA	C5-C3	2.03	1.55	1.51
14	A5	814	CLA	C1C-C2C	2.03	1.48	1.44
14	B2	838	CLA	C3D-C2D	2.03	1.43	1.39
14	A4	836	CLA	C3C-C2C	2.03	1.41	1.36
14	B6	826	CLA	C3C-C2C	2.03	1.41	1.36
14	A4	826	CLA	C5-C3	2.03	1.55	1.51
15	B3	1844	PQN	C11-C12	2.03	1.53	1.50
14	B2	814	CLA	C3C-C2C	2.03	1.41	1.36
14	A1	809	CLA	C1C-C2C	2.03	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B1	817	CLA	C3C-C2C	2.03	1.41	1.36
16	B5	1846	BCR	C26-C25	2.03	1.37	1.34
14	F1	1301	CLA	C3C-C2C	2.03	1.41	1.36
14	A4	803	CLA	O2A-CGA	2.03	1.39	1.33
16	B6	843	BCR	C1-C6	2.03	1.56	1.53
14	L3	203	CLA	O2A-CGA	2.03	1.39	1.33
14	A1	824	CLA	C1C-C2C	2.03	1.48	1.44
14	B2	838	CLA	O2A-CGA	2.03	1.39	1.33
14	B4	852	CLA	C1C-C2C	2.03	1.48	1.44
16	J1	103	BCR	C30-C25	2.03	1.56	1.53
14	A5	818	CLA	C3C-C2C	2.03	1.41	1.36
14	A4	853	CLA	C1C-C2C	2.03	1.48	1.44
14	B6	830	CLA	C3C-C2C	2.04	1.41	1.36
14	B2	838	CLA	C3C-C2C	2.04	1.41	1.36
14	A6	1625	CLA	C1C-C2C	2.04	1.48	1.44
16	J2	103	BCR	C30-C25	2.04	1.56	1.53
14	B3	1838	CLA	C1C-C2C	2.04	1.48	1.44
14	B6	836	CLA	C1C-C2C	2.04	1.48	1.44
15	B1	842	PQN	C11-C12	2.04	1.53	1.50
14	M6	1201	CLA	C3C-C2C	2.04	1.41	1.36
14	A2	1642	CLA	C3C-C2C	2.04	1.41	1.36
16	J2	102	BCR	C1-C6	2.04	1.56	1.53
14	A5	830	CLA	C1C-C2C	2.04	1.48	1.44
16	B3	1851	BCR	C5-C6	2.04	1.37	1.34
14	B3	1837	CLA	C1C-C2C	2.04	1.48	1.44
14	A6	1629	CLA	C3C-C2C	2.04	1.41	1.36
14	A3	843	CLA	C3C-C2C	2.04	1.41	1.36
14	J6	1103	CLA	C1C-C2C	2.04	1.48	1.44
14	L4	205	CLA	C3C-C2C	2.04	1.41	1.36
14	A5	842	CLA	C3C-C2C	2.04	1.41	1.36
14	A6	1616	CLA	C1C-C2C	2.04	1.48	1.44
14	A5	827	CLA	OBD-CAD	2.04	1.25	1.22
14	B4	818	CLA	C3C-C2C	2.04	1.41	1.36
14	A3	818	CLA	C3C-C2C	2.04	1.41	1.36
14	B2	817	CLA	C3C-C2C	2.04	1.41	1.36
14	X2	1701	CLA	C1C-C2C	2.04	1.48	1.44
14	F3	202	CLA	C1C-C2C	2.04	1.48	1.44
14	B2	815	CLA	C3C-C2C	2.04	1.41	1.36
14	B4	838	CLA	C1C-C2C	2.04	1.48	1.44
14	A2	1606	CLA	C3D-C2D	2.04	1.43	1.39
14	B5	1817	CLA	C3C-C2C	2.04	1.41	1.36
14	I1	101	CLA	C3D-C2D	2.04	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A2	1637	CLA	C1C-C2C	2.04	1.48	1.44
16	A6	1647	BCR	C1-C6	2.05	1.56	1.53
14	B3	1808	CLA	C3D-C2D	2.05	1.43	1.39
14	B4	831	CLA	O2D-CGD	2.05	1.38	1.33
14	L1	206	CLA	O2A-CGA	2.05	1.39	1.33
14	A3	843	CLA	O2D-CGD	2.05	1.38	1.33
14	A5	816	CLA	C1C-C2C	2.05	1.48	1.44
16	A3	852	BCR	C1-C6	2.05	1.56	1.53
14	A6	1627	CLA	OBD-CAD	2.05	1.25	1.22
14	A1	816	CLA	C3D-C2D	2.05	1.43	1.39
14	B2	817	CLA	O2A-CGA	2.05	1.39	1.33
14	A5	836	CLA	OBD-CAD	2.05	1.25	1.22
16	B6	847	BCR	C30-C25	2.05	1.56	1.53
16	B3	1846	BCR	C30-C25	2.05	1.56	1.53
14	B6	819	CLA	C1C-C2C	2.05	1.48	1.44
14	A6	1614	CLA	C1C-C2C	2.05	1.48	1.44
16	B6	845	BCR	C5-C6	2.05	1.38	1.34
14	A3	819	CLA	C3C-C2C	2.05	1.41	1.36
14	B3	1801	CLA	C1C-C2C	2.05	1.48	1.44
14	A4	808	CLA	C3D-C2D	2.05	1.43	1.39
14	A2	1631	CLA	C3C-C2C	2.05	1.41	1.36
14	L2	207	CLA	C1C-C2C	2.05	1.48	1.44
14	A4	839	CLA	C3C-C2C	2.05	1.41	1.36
16	F3	201	BCR	C5-C6	2.05	1.38	1.34
14	A2	1613	CLA	C3C-C2C	2.06	1.41	1.36
14	A3	830	CLA	C1C-C2C	2.06	1.48	1.44
14	A6	1632	CLA	OBD-CAD	2.06	1.25	1.22
14	A3	823	CLA	C3C-C2C	2.06	1.41	1.36
14	A4	818	CLA	C3C-C2C	2.06	1.41	1.36
14	B1	820	CLA	C1C-C2C	2.06	1.48	1.44
14	A6	1628	CLA	C3D-C2D	2.06	1.43	1.39
14	B2	829	CLA	C3C-C2C	2.06	1.41	1.36
14	A4	818	CLA	C3B-C2B	2.06	1.43	1.40
16	B2	846	BCR	C30-C25	2.06	1.56	1.53
14	A3	837	CLA	C3D-C2D	2.06	1.43	1.39
14	A4	815	CLA	C1C-C2C	2.06	1.48	1.44
16	B2	844	BCR	C1-C6	2.06	1.56	1.53
14	B4	829	CLA	C3C-C2C	2.06	1.41	1.36
14	L3	202	CLA	C1C-C2C	2.06	1.48	1.44
14	B1	815	CLA	C1C-C2C	2.06	1.48	1.44
14	B6	804	CLA	C3C-C2C	2.06	1.41	1.36
14	A1	806	CLA	C3D-C2D	2.06	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A1	826	CLA	C3D-C2D	2.06	1.43	1.39
14	B2	814	CLA	C3D-C2D	2.06	1.43	1.39
14	A3	837	CLA	OBD-CAD	2.06	1.25	1.22
14	A4	841	CLA	C3C-C2C	2.06	1.41	1.36
14	A5	829	CLA	C3C-C2C	2.06	1.41	1.36
14	A4	813	CLA	C1C-C2C	2.06	1.48	1.44
14	B6	815	CLA	C3D-C2D	2.06	1.43	1.39
16	A3	851	BCR	C1-C6	2.06	1.56	1.53
14	B5	1829	CLA	C3D-C2D	2.07	1.43	1.39
14	A3	816	CLA	C1C-C2C	2.07	1.48	1.44
14	B3	1818	CLA	C3C-C2C	2.07	1.41	1.36
14	L4	203	CLA	O2A-CGA	2.07	1.39	1.33
14	A4	841	CLA	O2D-CGD	2.07	1.38	1.33
14	A3	827	CLA	OBD-CAD	2.07	1.25	1.22
14	J4	102	CLA	C1C-C2C	2.07	1.48	1.44
14	F4	202	CLA	C3C-C2C	2.07	1.41	1.36
14	A5	839	CLA	C3D-C2D	2.07	1.43	1.39
14	B2	801	CLA	C3C-C2C	2.07	1.41	1.36
14	B3	1829	CLA	C3C-C2C	2.07	1.41	1.36
14	B4	841	CLA	C3C-C2C	2.07	1.41	1.36
14	A2	1601	CLA	C3D-C2D	2.07	1.43	1.39
14	A3	828	CLA	C3C-C2C	2.07	1.41	1.36
14	A3	825	CLA	C1C-C2C	2.07	1.48	1.44
14	A4	838	CLA	C3D-C2D	2.07	1.43	1.39
14	L6	208	CLA	C1C-C2C	2.07	1.48	1.44
16	A2	1652	BCR	C30-C25	2.07	1.56	1.53
14	A6	1617	CLA	C3D-C2D	2.07	1.43	1.39
14	A6	1627	CLA	C3D-C2D	2.07	1.43	1.39
14	L2	206	CLA	O2A-CGA	2.07	1.39	1.33
14	B1	801	CLA	C4C-C3C	2.07	1.48	1.45
14	A1	839	CLA	C1C-C2C	2.07	1.48	1.44
14	F2	204	CLA	C1C-C2C	2.07	1.48	1.44
16	A2	1651	BCR	C1-C6	2.07	1.56	1.53
14	A1	830	CLA	O2A-CGA	2.07	1.39	1.33
14	B5	1838	CLA	C1C-C2C	2.07	1.48	1.44
14	B3	1831	CLA	C3C-C2C	2.07	1.41	1.36
14	B3	1804	CLA	O2D-CGD	2.07	1.38	1.33
16	F1	1302	BCR	C30-C25	2.08	1.56	1.53
14	A2	1610	CLA	O2A-CGA	2.08	1.39	1.33
14	A6	1628	CLA	CHB-C4A	2.08	1.36	1.33
14	A2	1618	CLA	C1C-C2C	2.08	1.48	1.44
14	A6	1636	CLA	OBD-CAD	2.08	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B1	806	CLA	CHB-C4A	2.08	1.36	1.33
14	B1	829	CLA	C1C-C2C	2.08	1.48	1.44
14	A5	835	CLA	C1C-C2C	2.08	1.48	1.44
16	B3	1845	BCR	C1-C6	2.08	1.56	1.53
14	A1	811	CLA	C3C-C2C	2.08	1.41	1.36
14	A6	1623	CLA	C3D-C2D	2.08	1.43	1.39
14	B6	839	CLA	O2A-CGA	2.08	1.39	1.33
14	A4	835	CLA	C3C-C2C	2.08	1.41	1.36
14	A1	803	CLA	C3D-C2D	2.08	1.43	1.39
14	B4	827	CLA	C3B-C2B	2.08	1.43	1.40
16	B1	844	BCR	C26-C25	2.08	1.38	1.34
16	B5	1849	BCR	C30-C25	2.08	1.56	1.53
14	X5	101	CLA	C1C-C2C	2.08	1.48	1.44
14	B4	841	CLA	O2A-CGA	2.08	1.39	1.33
14	A2	1644	CLA	C3C-C2C	2.08	1.41	1.36
14	B6	827	CLA	C3C-C2C	2.08	1.41	1.36
14	B1	830	CLA	O2D-CGD	2.08	1.38	1.33
14	K6	1401	CLA	C1C-C2C	2.08	1.48	1.44
14	M2	1201	CLA	C3D-C2D	2.08	1.43	1.39
14	A2	1627	CLA	C1C-C2C	2.08	1.48	1.44
14	B3	1841	CLA	C3D-C2D	2.08	1.43	1.39
14	L6	207	CLA	C3D-C2D	2.09	1.43	1.39
16	J6	1105	BCR	C29-C30	2.09	1.58	1.54
14	B1	838	CLA	O2A-CGA	2.09	1.39	1.33
14	A5	808	CLA	C1C-C2C	2.09	1.48	1.44
14	K2	1401	CLA	C1C-C2C	2.09	1.48	1.44
14	A6	1635	CLA	C3C-C2C	2.09	1.41	1.36
14	A3	833	CLA	C3D-C2D	2.09	1.43	1.39
14	A3	826	CLA	C3C-C2C	2.09	1.41	1.36
14	A4	829	CLA	C1C-C2C	2.09	1.48	1.44
14	L6	203	CLA	C3C-C2C	2.09	1.41	1.36
14	B2	837	CLA	C1C-C2C	2.09	1.48	1.44
14	A2	1606	CLA	O2A-CGA	2.09	1.39	1.33
16	J2	103	BCR	C29-C30	2.09	1.59	1.54
16	J4	104	BCR	C29-C30	2.09	1.59	1.54
14	A3	812	CLA	C3C-C2C	2.09	1.41	1.36
14	A4	833	CLA	C3D-C2D	2.09	1.43	1.39
14	A6	1618	CLA	C3C-C2C	2.09	1.41	1.36
14	A1	818	CLA	C3C-C2C	2.09	1.41	1.36
14	A6	1632	CLA	C3D-C2D	2.09	1.43	1.39
14	B1	836	CLA	C1C-C2C	2.09	1.48	1.44
14	B5	1829	CLA	C3C-C2C	2.09	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B1	828	CLA	C3D-C2D	2.09	1.43	1.39
14	J6	1102	CLA	C1C-C2C	2.09	1.48	1.44
14	M1	1201	CLA	C3C-C2C	2.09	1.41	1.36
14	B1	837	CLA	C1C-C2C	2.09	1.48	1.44
14	B2	804	CLA	C3C-C2C	2.09	1.41	1.36
14	B2	803	CLA	O2A-CGA	2.09	1.39	1.33
14	A5	833	CLA	C3D-C2D	2.09	1.43	1.39
14	B5	1804	CLA	O2D-CGD	2.09	1.38	1.33
16	B3	1847	BCR	C1-C6	2.09	1.56	1.53
14	A6	1601	CLA	C1C-C2C	2.10	1.48	1.44
14	K5	102	CLA	C1C-C2C	2.10	1.48	1.44
14	A3	804	CLA	O2A-CGA	2.10	1.39	1.33
14	A2	1633	CLA	C3D-C2D	2.10	1.43	1.39
14	A5	824	CLA	C3D-C2D	2.10	1.43	1.39
14	B3	1826	CLA	CHB-C4A	2.10	1.36	1.33
14	A2	1630	CLA	C3D-C2D	2.10	1.43	1.39
16	J4	103	BCR	C30-C25	2.10	1.56	1.53
14	A5	827	CLA	C3D-C2D	2.10	1.43	1.39
14	B6	833	CLA	C3D-C2D	2.10	1.43	1.39
14	B4	820	CLA	O2A-CGA	2.10	1.39	1.33
14	L4	204	CLA	O2A-CGA	2.10	1.39	1.33
14	L3	204	CLA	O2A-CGA	2.10	1.39	1.33
14	X5	101	CLA	C3C-C2C	2.10	1.41	1.36
16	B6	845	BCR	C1-C6	2.10	1.56	1.53
14	L6	206	CLA	O2A-CGA	2.10	1.39	1.33
14	B6	827	CLA	C3D-C2D	2.10	1.43	1.39
14	B3	1815	CLA	C3B-C2B	2.10	1.43	1.40
14	A1	828	CLA	C3C-C2C	2.10	1.41	1.36
14	A3	833	CLA	C3C-C2C	2.10	1.41	1.36
16	A3	848	BCR	C30-C25	2.10	1.56	1.53
14	B6	828	CLA	C3D-C2D	2.10	1.43	1.39
14	A1	809	CLA	C3D-C2D	2.10	1.43	1.39
14	A2	1637	CLA	C3C-C2C	2.10	1.41	1.36
14	B6	829	CLA	C3C-C2C	2.10	1.41	1.36
16	J5	104	BCR	C29-C30	2.10	1.59	1.54
16	A5	850	BCR	C1-C6	2.10	1.56	1.53
16	A3	852	BCR	C30-C25	2.10	1.56	1.53
14	B5	1841	CLA	O2A-CGA	2.10	1.39	1.33
14	A4	815	CLA	C3C-C2C	2.10	1.41	1.36
14	A6	1608	CLA	O2A-CGA	2.10	1.39	1.33
14	A4	818	CLA	C3B-CAB	2.10	1.52	1.47
14	B4	827	CLA	C3D-C2D	2.10	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B5	1807	CLA	C3C-C2C	2.11	1.41	1.36
14	B5	1827	CLA	C3B-C2B	2.11	1.43	1.40
14	B1	853	CLA	C1C-C2C	2.11	1.48	1.44
14	A3	809	CLA	C3D-C2D	2.11	1.43	1.39
14	B2	835	CLA	C1C-C2C	2.11	1.48	1.44
14	A3	836	CLA	C3C-C2C	2.11	1.41	1.36
14	B4	839	CLA	O2A-CGA	2.11	1.39	1.33
14	L5	202	CLA	C1C-C2C	2.11	1.48	1.44
14	A4	828	CLA	C3C-C2C	2.11	1.41	1.36
14	L3	205	CLA	C1C-C2C	2.11	1.48	1.44
14	A3	810	CLA	C3D-C2D	2.11	1.43	1.39
14	B3	1803	CLA	C3C-C2C	2.11	1.41	1.36
16	J3	104	BCR	C29-C30	2.11	1.59	1.54
14	A5	817	CLA	C3D-C2D	2.11	1.43	1.39
14	A5	841	CLA	C1-C2	2.11	1.55	1.49
14	A2	1641	CLA	C3D-C2D	2.11	1.43	1.39
14	B3	1840	CLA	C1C-C2C	2.11	1.48	1.44
14	A4	834	CLA	C1C-C2C	2.11	1.48	1.44
14	J1	102	CLA	C1C-C2C	2.11	1.48	1.44
14	B1	841	CLA	C3C-C2C	2.11	1.41	1.36
14	B6	817	CLA	O2A-CGA	2.11	1.39	1.33
14	B3	1841	CLA	O2A-CGA	2.11	1.39	1.33
14	A3	845	CLA	C1C-C2C	2.11	1.48	1.44
14	A2	1634	CLA	C3C-C2C	2.11	1.41	1.36
14	B5	1832	CLA	C3C-C2C	2.12	1.41	1.36
14	A3	842	CLA	C1-C2	2.12	1.55	1.49
14	L5	206	CLA	C3C-C2C	2.12	1.41	1.36
14	A3	824	CLA	C3D-C2D	2.12	1.43	1.39
14	A1	810	CLA	C3C-C2C	2.12	1.41	1.36
14	B2	808	CLA	O2A-CGA	2.12	1.39	1.33
14	A4	812	CLA	C3C-C2C	2.12	1.41	1.36
14	A1	817	CLA	C3C-C2C	2.12	1.41	1.36
14	B2	832	CLA	C3D-C2D	2.12	1.43	1.39
14	B3	1806	CLA	C3C-C2C	2.12	1.41	1.36
14	B5	1843	CLA	C3C-C2C	2.12	1.41	1.36
14	B6	818	CLA	O2A-CGA	2.12	1.39	1.33
14	B2	813	CLA	O2A-CGA	2.12	1.39	1.33
14	A3	805	CLA	C3C-C2C	2.12	1.41	1.36
14	A6	1637	CLA	O2D-CGD	2.12	1.38	1.33
14	B5	1821	CLA	C1C-C2C	2.12	1.48	1.44
14	B4	816	CLA	O2A-CGA	2.12	1.39	1.33
14	B5	1806	CLA	C3D-C2D	2.12	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A2	1626	CLA	C3D-C2D	2.12	1.43	1.39
14	B4	817	CLA	C3D-C2D	2.12	1.43	1.39
16	A4	849	BCR	C1-C6	2.12	1.56	1.53
16	B6	844	BCR	C30-C25	2.12	1.56	1.53
14	A3	844	CLA	C3C-C2C	2.12	1.41	1.36
14	L1	207	CLA	C3C-C2C	2.12	1.41	1.36
14	B5	1841	CLA	C3C-C2C	2.12	1.41	1.36
14	A3	808	CLA	O2A-CGA	2.12	1.39	1.33
14	A3	803	CLA	O2D-CGD	2.12	1.38	1.33
14	A6	1651	CLA	O2D-CGD	2.12	1.38	1.33
14	B2	818	CLA	C1C-C2C	2.12	1.48	1.44
14	B4	812	CLA	O2D-CGD	2.12	1.38	1.33
14	A4	823	CLA	C3D-C2D	2.12	1.43	1.39
14	A3	840	CLA	C3D-C2D	2.12	1.43	1.39
14	A4	840	CLA	C1-C2	2.12	1.55	1.49
14	X4	102	CLA	C1C-C2C	2.12	1.48	1.44
14	A4	816	CLA	C3D-C2D	2.12	1.43	1.39
14	B4	806	CLA	C3D-C2D	2.12	1.43	1.39
16	B2	843	BCR	C30-C25	2.12	1.56	1.53
14	A1	839	CLA	C3C-C2C	2.12	1.41	1.36
14	B1	827	CLA	C3C-C2C	2.12	1.41	1.36
14	L2	207	CLA	O2D-CGD	2.12	1.38	1.33
14	B1	840	CLA	O2A-CGA	2.12	1.39	1.33
14	L2	206	CLA	C3D-C2D	2.12	1.43	1.39
14	B1	840	CLA	C3D-C2D	2.13	1.43	1.39
16	A2	1652	BCR	C1-C6	2.13	1.56	1.53
14	L1	207	CLA	C1C-C2C	2.13	1.48	1.44
14	A4	835	CLA	C3D-C2D	2.13	1.43	1.39
14	B1	809	CLA	C3C-C2C	2.13	1.41	1.36
14	L4	201	CLA	OBD-CAD	2.13	1.25	1.22
14	A6	1627	CLA	C3C-C2C	2.13	1.41	1.36
14	B6	805	CLA	C4C-C3C	2.13	1.48	1.45
14	A3	817	CLA	C3D-C2D	2.13	1.44	1.39
14	A3	807	CLA	C3C-C2C	2.13	1.41	1.36
16	B4	846	BCR	C26-C25	2.13	1.38	1.34
16	A6	1644	BCR	C30-C25	2.13	1.56	1.53
14	L2	202	CLA	OBD-CAD	2.13	1.25	1.22
14	B2	823	CLA	C1C-C2C	2.13	1.48	1.44
14	B1	805	CLA	O2D-CGD	2.13	1.38	1.33
14	B5	1830	CLA	C3D-C2D	2.13	1.44	1.39
16	M3	1602	BCR	C1-C6	2.13	1.56	1.53
14	B6	841	CLA	C3C-C2C	2.13	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A1	838	CLA	C1-C2	2.13	1.55	1.49
14	B5	1828	CLA	C3B-C2B	2.13	1.43	1.40
14	B2	827	CLA	C3D-C2D	2.13	1.44	1.39
14	B6	823	CLA	C1C-C2C	2.13	1.48	1.44
14	A3	832	CLA	C3C-C2C	2.13	1.41	1.36
14	A4	827	CLA	C3D-C2D	2.13	1.44	1.39
14	A6	1630	CLA	O2A-CGA	2.13	1.39	1.33
14	B3	1820	CLA	O2A-CGA	2.13	1.39	1.33
16	B1	844	BCR	C30-C25	2.13	1.56	1.53
14	B4	809	CLA	O2A-CGA	2.13	1.39	1.33
14	B5	1819	CLA	C3D-C2D	2.13	1.44	1.39
14	K4	1401	CLA	C1C-C2C	2.13	1.48	1.44
14	B6	835	CLA	C1C-C2C	2.13	1.48	1.44
14	B4	843	CLA	C3C-C2C	2.13	1.41	1.36
14	A6	1640	CLA	C1-C2	2.13	1.55	1.49
14	K1	1401	CLA	C1C-C2C	2.13	1.48	1.44
14	A2	1638	CLA	C3D-C2D	2.13	1.44	1.39
14	B6	809	CLA	O2A-CGA	2.13	1.39	1.33
14	A1	829	CLA	O2A-CGA	2.13	1.39	1.33
16	B6	850	BCR	C1-C6	2.13	1.56	1.53
14	M3	1601	CLA	C1C-C2C	2.13	1.48	1.44
14	A2	1641	CLA	O2A-CGA	2.13	1.39	1.33
14	L5	205	CLA	O2A-CGA	2.13	1.39	1.33
16	B6	844	BCR	C26-C25	2.13	1.38	1.34
14	A2	1632	CLA	O2A-CGA	2.14	1.39	1.33
14	I1	101	CLA	C3C-C2C	2.14	1.41	1.36
14	B3	1816	CLA	O2A-CGA	2.14	1.39	1.33
14	A5	842	CLA	O2D-CGD	2.14	1.38	1.33
14	B3	1815	CLA	O2A-CGA	2.14	1.39	1.33
14	B5	1801	CLA	C1C-C2C	2.14	1.48	1.44
14	B4	807	CLA	C3C-C2C	2.14	1.41	1.36
14	A2	1612	CLA	C3D-C2D	2.14	1.44	1.39
14	B5	1806	CLA	C3C-C2C	2.14	1.41	1.36
14	A3	834	CLA	OBD-CAD	2.14	1.25	1.22
14	L6	203	CLA	O2D-CGD	2.14	1.38	1.33
14	B1	826	CLA	O2D-CGD	2.14	1.38	1.33
14	B2	825	CLA	C3B-C2B	2.14	1.43	1.40
14	B4	825	CLA	C1C-C2C	2.14	1.48	1.44
14	A6	1635	CLA	C1C-C2C	2.14	1.48	1.44
14	A2	1633	CLA	O2A-CGA	2.14	1.39	1.33
14	A2	1629	CLA	C3D-C2D	2.14	1.44	1.39
14	B1	824	CLA	C3C-C2C	2.14	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A3	839	CLA	C3C-C2C	2.14	1.41	1.36
14	A5	808	CLA	O2A-CGA	2.14	1.39	1.33
14	A5	833	CLA	OBD-CAD	2.14	1.25	1.22
14	B6	838	CLA	C1C-C2C	2.14	1.48	1.44
14	B5	1808	CLA	C3D-C2D	2.14	1.44	1.39
14	B5	1839	CLA	O2A-CGA	2.14	1.39	1.33
14	A2	1645	CLA	C3C-C2C	2.14	1.41	1.36
14	B3	1809	CLA	O2A-CGA	2.14	1.39	1.33
14	B6	814	CLA	O2A-CGA	2.14	1.39	1.33
14	B4	840	CLA	C1C-C2C	2.14	1.48	1.44
14	A1	803	CLA	O2A-CGA	2.14	1.39	1.33
14	B3	1831	CLA	O2A-CGA	2.14	1.39	1.33
14	A3	828	CLA	CHB-C4A	2.14	1.36	1.33
14	A5	843	CLA	C3C-C2C	2.14	1.41	1.36
14	A5	823	CLA	C3D-C2D	2.14	1.44	1.39
14	B3	1825	CLA	C1C-C2C	2.14	1.48	1.44
14	B3	1839	CLA	O2D-CGD	2.14	1.38	1.33
14	A3	838	CLA	O2D-CGD	2.14	1.38	1.33
14	L6	202	CLA	C3C-C2C	2.14	1.41	1.36
14	B3	1806	CLA	C3D-C2D	2.14	1.44	1.39
14	B6	804	CLA	C1C-C2C	2.14	1.48	1.44
14	B3	1828	CLA	OBD-CAD	2.14	1.25	1.22
14	A4	834	CLA	C3C-C2C	2.14	1.41	1.36
16	J1	104	BCR	C29-C30	2.14	1.59	1.54
14	B6	824	CLA	CHB-C4A	2.14	1.36	1.33
14	L2	205	CLA	O2A-CGA	2.14	1.39	1.33
14	B4	836	CLA	O2D-CGD	2.14	1.38	1.33
14	J3	102	CLA	C1C-C2C	2.14	1.48	1.44
14	A5	807	CLA	C3C-C2C	2.14	1.41	1.36
14	B6	833	CLA	C3C-C2C	2.14	1.41	1.36
14	B3	1832	CLA	C3D-C2D	2.14	1.44	1.39
14	B2	840	CLA	C3C-C2C	2.15	1.41	1.36
16	M5	101	BCR	C1-C6	2.15	1.56	1.53
16	J5	105	BCR	C5-C6	2.15	1.38	1.34
14	A2	1621	CLA	C3C-C2C	2.15	1.41	1.36
14	B4	824	CLA	C3B-C2B	2.15	1.43	1.40
14	B2	816	CLA	O2A-CGA	2.15	1.39	1.33
14	A3	827	CLA	C3C-C2C	2.15	1.41	1.36
14	B2	812	CLA	O2A-CGA	2.15	1.39	1.33
14	A3	807	CLA	C3D-C2D	2.15	1.44	1.39
14	B6	826	CLA	C3B-C2B	2.15	1.43	1.40
14	B3	1834	CLA	C3D-C2D	2.15	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A2	1639	CLA	O2D-CGD	2.15	1.38	1.33
16	M2	1202	BCR	C1-C6	2.15	1.56	1.53
14	B4	803	CLA	C3C-C2C	2.15	1.41	1.36
14	A5	843	CLA	C1C-C2C	2.15	1.48	1.44
14	A6	1607	CLA	C3C-C2C	2.15	1.41	1.36
14	B1	806	CLA	O2A-CGA	2.15	1.39	1.33
14	B3	1816	CLA	C3D-C2D	2.15	1.44	1.39
14	A5	827	CLA	C3C-C2C	2.15	1.41	1.36
14	A4	829	CLA	O2A-CGA	2.15	1.39	1.33
14	A2	1629	CLA	C3C-C2C	2.15	1.41	1.36
14	B2	825	CLA	OBD-CAD	2.15	1.25	1.22
14	A5	825	CLA	C1C-C2C	2.15	1.48	1.44
14	A5	811	CLA	O2A-CGA	2.15	1.39	1.33
14	B3	1807	CLA	C3C-C2C	2.15	1.41	1.36
14	A2	1614	CLA	C3C-C2C	2.15	1.41	1.36
14	A4	807	CLA	O2A-CGA	2.15	1.39	1.33
14	A4	817	CLA	C3C-C2C	2.15	1.41	1.36
14	B6	807	CLA	C3D-C2D	2.15	1.44	1.39
14	A3	832	CLA	OBD-CAD	2.15	1.25	1.22
14	K3	1401	CLA	C1C-C2C	2.15	1.48	1.44
14	A4	809	CLA	C3D-C2D	2.15	1.44	1.39
14	A2	1629	CLA	OBD-CAD	2.15	1.25	1.22
14	A6	1628	CLA	C3C-C2C	2.15	1.41	1.36
14	B1	833	CLA	C3D-C2D	2.15	1.44	1.39
14	B5	1820	CLA	C3D-C2D	2.16	1.44	1.39
14	B2	802	CLA	O2D-CGD	2.16	1.38	1.33
14	B1	828	CLA	C3C-C2C	2.16	1.41	1.36
14	A6	1612	CLA	C3C-C2C	2.16	1.41	1.36
14	A2	1630	CLA	C3C-C2C	2.16	1.41	1.36
14	A5	836	CLA	O2D-CGD	2.16	1.38	1.33
14	A1	802	CLA	O2D-CGD	2.16	1.38	1.33
14	B4	815	CLA	O2A-CGA	2.16	1.39	1.33
14	A6	1631	CLA	O2A-CGA	2.16	1.39	1.33
14	J4	101	CLA	C1C-C2C	2.16	1.48	1.44
14	A1	807	CLA	O2A-CGA	2.16	1.39	1.33
14	X4	102	CLA	O2D-CGD	2.16	1.38	1.33
14	B3	1805	CLA	O2D-CGD	2.16	1.38	1.33
14	A5	805	CLA	C3D-C2D	2.16	1.44	1.39
14	A4	830	CLA	O2A-CGA	2.16	1.39	1.33
14	A5	830	CLA	O2A-CGA	2.16	1.39	1.33
14	B6	829	CLA	O2D-CGD	2.16	1.38	1.33
14	B4	832	CLA	C3C-C2C	2.16	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X2	1701	CLA	C3C-C2C	2.16	1.41	1.36
14	B5	1809	CLA	O2A-CGA	2.16	1.39	1.33
14	A5	812	CLA	C3C-C2C	2.16	1.41	1.36
14	A6	1604	CLA	O2A-CGA	2.16	1.39	1.33
14	A3	837	CLA	O2D-CGD	2.16	1.38	1.33
14	A3	831	CLA	C3D-C2D	2.16	1.44	1.39
14	A6	1633	CLA	OBD-CAD	2.16	1.25	1.22
14	L5	206	CLA	C1C-C2C	2.16	1.48	1.44
14	A5	828	CLA	C3D-C2D	2.16	1.44	1.39
14	A1	827	CLA	C3D-C2D	2.16	1.44	1.39
14	B1	825	CLA	CHB-C4A	2.16	1.36	1.33
14	A3	835	CLA	C3D-C2D	2.16	1.44	1.39
14	B2	828	CLA	O2D-CGD	2.16	1.38	1.33
14	A5	833	CLA	C3C-C2C	2.16	1.41	1.36
14	A2	1635	CLA	C3C-C2C	2.16	1.41	1.36
14	L1	205	CLA	O2A-CGA	2.16	1.39	1.33
14	B2	836	CLA	O2D-CGD	2.16	1.38	1.33
14	B4	835	CLA	C3C-C2C	2.16	1.41	1.36
14	A2	1643	CLA	C1-C2	2.17	1.55	1.49
14	B5	1842	CLA	O2D-CGD	2.17	1.38	1.33
14	A4	832	CLA	OBD-CAD	2.17	1.25	1.22
14	A2	1636	CLA	C3C-C2C	2.17	1.41	1.36
14	A4	824	CLA	C1C-C2C	2.17	1.48	1.44
14	A5	831	CLA	O2A-CGA	2.17	1.39	1.33
14	B4	806	CLA	C3C-C2C	2.17	1.41	1.36
14	A5	836	CLA	C3D-C2D	2.17	1.44	1.39
14	A6	1636	CLA	C3D-C2D	2.17	1.44	1.39
14	A4	826	CLA	OBD-CAD	2.17	1.25	1.22
14	L1	205	CLA	OBD-CAD	2.17	1.25	1.22
14	A5	809	CLA	C3C-C2C	2.17	1.41	1.36
14	B4	810	CLA	C3C-C2C	2.17	1.41	1.36
14	A1	808	CLA	C3D-C2D	2.17	1.44	1.39
14	B6	837	CLA	O2A-CGA	2.17	1.39	1.33
14	B5	1835	CLA	C3C-C2C	2.17	1.41	1.36
14	L5	204	CLA	O2A-CGA	2.17	1.39	1.33
14	A1	832	CLA	C3C-C2C	2.17	1.41	1.36
14	A4	802	CLA	O2D-CGD	2.17	1.38	1.33
16	B2	850	BCR	C1-C6	2.17	1.56	1.53
14	B3	1820	CLA	C3D-C2D	2.17	1.44	1.39
14	A4	803	CLA	C3D-C2D	2.17	1.44	1.39
14	B2	825	CLA	C3D-C2D	2.17	1.44	1.39
14	A2	1620	CLA	C3C-C2C	2.17	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B3	1843	CLA	C3C-C2C	2.17	1.41	1.36
14	B5	1840	CLA	C1C-C2C	2.17	1.48	1.44
14	A4	830	CLA	C3D-C2D	2.17	1.44	1.39
16	A6	1648	BCR	C30-C25	2.17	1.56	1.53
14	B1	814	CLA	O2A-CGA	2.17	1.39	1.33
14	L4	205	CLA	O2D-CGD	2.17	1.38	1.33
14	B3	1839	CLA	O2A-CGA	2.17	1.39	1.33
16	B2	842	BCR	C1-C6	2.17	1.56	1.53
14	A5	814	CLA	C3C-C2C	2.17	1.41	1.36
14	A5	823	CLA	C3C-C2C	2.17	1.41	1.36
14	L1	201	CLA	OBD-CAD	2.17	1.25	1.22
14	J6	1101	CLA	O2D-CGD	2.17	1.38	1.33
14	B1	811	CLA	O2A-CGA	2.17	1.39	1.33
14	A3	809	CLA	C3C-C2C	2.17	1.41	1.36
14	B5	1831	CLA	O2D-CGD	2.17	1.38	1.33
14	X3	102	CLA	C1C-C2C	2.17	1.48	1.44
14	A5	803	CLA	C3D-C2D	2.17	1.44	1.39
14	B4	830	CLA	C3D-C2D	2.17	1.44	1.39
14	A1	819	CLA	C3D-C2D	2.17	1.44	1.39
14	A5	803	CLA	O2D-CGD	2.17	1.38	1.33
14	K3	1401	CLA	C3C-C2C	2.17	1.41	1.36
14	A6	1619	CLA	C3C-C2C	2.18	1.41	1.36
14	A4	826	CLA	C3C-C2C	2.18	1.41	1.36
14	B1	830	CLA	O2A-CGA	2.18	1.39	1.33
14	A2	1623	CLA	C3D-C2D	2.18	1.44	1.39
14	B5	1837	CLA	C1C-C2C	2.18	1.48	1.44
14	A1	833	CLA	C3C-C2C	2.18	1.41	1.36
14	B5	1819	CLA	O2A-CGA	2.18	1.39	1.33
16	B1	852	BCR	C5-C6	2.18	1.38	1.34
14	A5	804	CLA	O2A-CGA	2.18	1.39	1.33
14	B3	1842	CLA	O2D-CGD	2.18	1.38	1.33
14	A2	1636	CLA	C3D-C2D	2.18	1.44	1.39
14	B2	836	CLA	O2A-CGA	2.18	1.39	1.33
14	L2	207	CLA	C3C-C2C	2.18	1.41	1.36
14	A2	1611	CLA	C3C-C2C	2.18	1.41	1.36
14	B6	832	CLA	C3D-C2D	2.18	1.44	1.39
14	L5	203	CLA	OBD-CAD	2.18	1.25	1.22
14	A3	831	CLA	O2A-CGA	2.18	1.39	1.33
14	A3	803	CLA	C3D-C2D	2.18	1.44	1.39
14	A1	836	CLA	C3C-C2C	2.18	1.41	1.36
14	A3	804	CLA	C3D-C2D	2.18	1.44	1.39
14	A5	834	CLA	C3D-C2D	2.18	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B1	819	CLA	O2A-CGA	2.18	1.39	1.33
14	B6	806	CLA	C3C-C2C	2.18	1.41	1.36
14	B1	807	CLA	C3C-C2C	2.18	1.41	1.36
14	B4	819	CLA	O2A-CGA	2.18	1.39	1.33
14	A4	811	CLA	C3C-C2C	2.18	1.41	1.36
14	X6	1701	CLA	C1C-C2C	2.18	1.48	1.44
14	B4	801	CLA	O2A-CGA	2.18	1.39	1.33
14	B3	1831	CLA	O2D-CGD	2.18	1.38	1.33
14	B4	852	CLA	C3C-C2C	2.18	1.41	1.36
14	A6	1639	CLA	C3D-C2D	2.18	1.44	1.39
14	A6	1632	CLA	C3C-C2C	2.18	1.41	1.36
14	B1	803	CLA	C3D-C2D	2.18	1.44	1.39
14	B2	832	CLA	C3C-C2C	2.18	1.41	1.36
14	B1	853	CLA	C3C-C2C	2.18	1.41	1.36
14	B1	810	CLA	C3C-C2C	2.19	1.41	1.36
14	K2	1401	CLA	C3C-C2C	2.19	1.41	1.36
14	B5	1815	CLA	O2A-CGA	2.19	1.39	1.33
14	B6	807	CLA	O2A-CGA	2.19	1.39	1.33
14	B1	803	CLA	O2A-CGA	2.19	1.39	1.33
14	B1	829	CLA	C3D-C2D	2.19	1.44	1.39
14	I6	101	CLA	O2A-CGA	2.19	1.39	1.33
14	B6	840	CLA	OBD-CAD	2.19	1.25	1.22
14	B1	801	CLA	OBD-CAD	2.19	1.25	1.22
16	B4	849	BCR	C30-C25	2.19	1.56	1.53
14	A4	836	CLA	O2D-CGD	2.19	1.38	1.33
14	A5	832	CLA	OBD-CAD	2.19	1.25	1.22
14	I6	101	CLA	C3C-C2C	2.19	1.41	1.36
14	B3	1813	CLA	C3D-C2D	2.19	1.44	1.39
14	L1	202	CLA	OBD-CAD	2.19	1.25	1.22
14	B5	1820	CLA	O2A-CGA	2.19	1.39	1.33
14	A1	835	CLA	O2D-CGD	2.19	1.38	1.33
14	X4	102	CLA	C3C-C2C	2.19	1.41	1.36
14	B1	816	CLA	C3D-C2D	2.19	1.44	1.39
14	B3	1804	CLA	O2A-CGA	2.19	1.39	1.33
14	B2	822	CLA	C3C-C2C	2.19	1.41	1.36
14	B1	824	CLA	O2D-CGD	2.19	1.38	1.33
14	A4	810	CLA	C3C-C2C	2.19	1.41	1.36
14	B5	1810	CLA	C3C-C2C	2.19	1.41	1.36
14	A6	1623	CLA	C3C-C2C	2.19	1.41	1.36
14	A1	807	CLA	C1C-C2C	2.19	1.48	1.44
14	A4	831	CLA	C3C-C2C	2.19	1.41	1.36
14	B2	801	CLA	C1C-C2C	2.19	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B2	831	CLA	O2D-CGD	2.19	1.38	1.33
14	A2	1604	CLA	C3D-C2D	2.19	1.44	1.39
14	A1	834	CLA	O2D-CGD	2.19	1.38	1.33
14	B3	1810	CLA	C3C-C2C	2.19	1.41	1.36
14	A4	827	CLA	C3C-C2C	2.19	1.41	1.36
14	A1	839	CLA	O2D-CGD	2.19	1.38	1.33
14	B2	831	CLA	C3D-C2D	2.19	1.44	1.39
14	L6	208	CLA	C3C-C2C	2.19	1.41	1.36
14	A1	834	CLA	OBD-CAD	2.19	1.25	1.22
14	A4	853	CLA	C3D-C2D	2.19	1.44	1.39
14	A6	1631	CLA	C3D-C2D	2.19	1.44	1.39
14	A3	808	CLA	C1C-C2C	2.20	1.48	1.44
14	A3	840	CLA	O2A-CGA	2.20	1.39	1.33
14	A6	1625	CLA	C3D-C2D	2.20	1.44	1.39
14	B2	805	CLA	C3C-C2C	2.20	1.41	1.36
14	L3	205	CLA	C3C-C2C	2.20	1.41	1.36
14	M1	1201	CLA	C3D-C2D	2.20	1.44	1.39
14	B4	808	CLA	C3D-C2D	2.20	1.44	1.39
14	A2	1625	CLA	C3C-C2C	2.20	1.41	1.36
14	B5	1803	CLA	C3C-C2C	2.20	1.41	1.36
14	B1	831	CLA	C3C-C2C	2.20	1.41	1.36
14	X1	1701	CLA	C3C-C2C	2.20	1.41	1.36
14	A2	1619	CLA	C3D-C2D	2.20	1.44	1.39
14	B5	1817	CLA	C3D-C2D	2.20	1.44	1.39
14	A1	806	CLA	C3C-C2C	2.20	1.41	1.36
14	B5	1803	CLA	C1C-C2C	2.20	1.48	1.44
14	B6	826	CLA	OBD-CAD	2.20	1.25	1.22
14	B1	818	CLA	O2A-CGA	2.20	1.39	1.33
14	A6	1651	CLA	O2A-CGA	2.20	1.39	1.33
14	L2	205	CLA	OBD-CAD	2.20	1.25	1.22
14	B4	835	CLA	C3D-C2D	2.20	1.44	1.39
14	A1	826	CLA	C3C-C2C	2.20	1.41	1.36
14	B4	837	CLA	C1C-C2C	2.20	1.48	1.44
14	A4	804	CLA	C3D-C2D	2.20	1.44	1.39
14	A2	1603	CLA	OBD-CAD	2.20	1.25	1.22
14	B2	834	CLA	C1C-C2C	2.20	1.48	1.44
14	J2	101	CLA	C1C-C2C	2.20	1.48	1.44
14	B2	835	CLA	C3C-C2C	2.20	1.41	1.36
14	B6	840	CLA	O2D-CGD	2.20	1.38	1.33
14	A5	837	CLA	O2D-CGD	2.20	1.38	1.33
14	A1	823	CLA	C3D-C2D	2.20	1.44	1.39
14	A6	1604	CLA	C3D-C2D	2.20	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	K5	101	CLA	C3C-C2C	2.20	1.41	1.36
14	B6	805	CLA	O2D-CGD	2.20	1.38	1.33
14	X3	102	CLA	C3C-C2C	2.21	1.41	1.36
14	A4	842	CLA	C3C-C2C	2.21	1.41	1.36
14	B1	839	CLA	C1C-C2C	2.21	1.48	1.44
14	B3	1811	CLA	O2A-CGA	2.21	1.39	1.33
14	B2	817	CLA	C3D-C2D	2.21	1.44	1.39
14	B4	838	CLA	C3C-C2C	2.21	1.41	1.36
14	B1	818	CLA	C3C-C2C	2.21	1.41	1.36
14	A4	819	CLA	C3D-C2D	2.21	1.44	1.39
14	J3	101	CLA	C1C-C2C	2.21	1.48	1.44
14	A3	805	CLA	C3D-C2D	2.21	1.44	1.39
14	B2	809	CLA	O2D-CGD	2.21	1.38	1.33
14	A1	840	CLA	C3C-C2C	2.21	1.41	1.36
14	A6	1634	CLA	C3C-C2C	2.21	1.41	1.36
14	A6	1610	CLA	C3C-C2C	2.21	1.41	1.36
14	B5	1816	CLA	O2A-CGA	2.21	1.39	1.33
14	B4	842	CLA	O2D-CGD	2.21	1.38	1.33
16	B4	847	BCR	C1-C6	2.21	1.56	1.53
14	A4	806	CLA	C3C-C2C	2.21	1.41	1.36
14	B4	839	CLA	O2D-CGD	2.21	1.38	1.33
16	B3	1846	BCR	C26-C25	2.21	1.38	1.34
14	A1	804	CLA	C3D-C2D	2.21	1.44	1.39
14	A4	833	CLA	C3C-C2C	2.21	1.41	1.36
16	A1	846	BCR	C1-C6	2.21	1.56	1.53
14	B3	1801	CLA	C3C-C2C	2.21	1.41	1.36
14	J5	101	CLA	C1C-C2C	2.21	1.48	1.44
17	X5	102	LHG	P-O4	2.21	1.66	1.55
14	B2	828	CLA	O2A-CGA	2.21	1.39	1.33
14	B5	1819	CLA	C3C-C2C	2.21	1.41	1.36
14	A2	1636	CLA	O2A-CGA	2.21	1.39	1.33
14	A4	832	CLA	C3D-C2D	2.21	1.44	1.39
14	A6	1609	CLA	C3C-C2C	2.22	1.41	1.36
14	L1	207	CLA	O2D-CGD	2.22	1.38	1.33
14	A3	821	CLA	C3D-C2D	2.22	1.44	1.39
14	A6	1605	CLA	C3C-C2C	2.22	1.41	1.36
14	B5	1809	CLA	C3C-C2C	2.22	1.41	1.36
14	B5	1831	CLA	O2A-CGA	2.22	1.39	1.33
14	A6	1638	CLA	C3C-C2C	2.22	1.41	1.36
14	A3	836	CLA	C1C-C2C	2.22	1.48	1.44
14	A5	835	CLA	C3D-C2D	2.22	1.44	1.39
16	J1	104	BCR	C30-C25	2.22	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B1	804	CLA	O2A-CGA	2.22	1.39	1.33
14	B3	1842	CLA	C3C-C2C	2.22	1.41	1.36
14	B2	807	CLA	C3C-C2C	2.22	1.41	1.36
14	B5	1842	CLA	C3C-C2C	2.22	1.41	1.36
14	B5	1812	CLA	O2D-CGD	2.22	1.38	1.33
14	B6	824	CLA	C1C-C2C	2.22	1.48	1.44
14	B4	813	CLA	C3D-C2D	2.22	1.44	1.39
14	A3	829	CLA	O2A-CGA	2.22	1.39	1.33
14	A6	1608	CLA	C1C-C2C	2.22	1.48	1.44
14	L3	204	CLA	C3D-C2D	2.22	1.44	1.39
14	B3	1829	CLA	C3D-C2D	2.22	1.44	1.39
14	A2	1640	CLA	O2A-CGA	2.22	1.39	1.33
14	A3	823	CLA	C3D-C2D	2.22	1.44	1.39
14	A3	845	CLA	C3C-C2C	2.22	1.41	1.36
14	B5	1811	CLA	O2A-CGA	2.22	1.39	1.33
14	B6	818	CLA	C3D-C2D	2.22	1.44	1.39
14	A2	1622	CLA	C3D-C2D	2.22	1.44	1.39
14	A3	802	CLA	OBD-CAD	2.22	1.25	1.22
14	B1	830	CLA	C3C-C2C	2.22	1.41	1.36
14	A5	802	CLA	OBD-CAD	2.22	1.25	1.22
14	B2	839	CLA	O2D-CGD	2.22	1.38	1.33
14	K5	102	CLA	C3C-C2C	2.22	1.41	1.36
14	L5	204	CLA	OBD-CAD	2.22	1.25	1.22
14	A5	826	CLA	C3C-C2C	2.22	1.41	1.36
14	A4	822	CLA	C3D-C2D	2.22	1.44	1.39
14	B3	1804	CLA	C3C-C2C	2.22	1.41	1.36
14	B5	1808	CLA	O2A-CGA	2.22	1.39	1.33
14	A1	823	CLA	O2A-CGA	2.22	1.39	1.33
14	B5	1828	CLA	C3D-C2D	2.22	1.44	1.39
14	A6	1616	CLA	C3D-C2D	2.22	1.44	1.39
14	A4	837	CLA	C3C-C2C	2.22	1.41	1.36
14	B3	1825	CLA	C3C-C2C	2.22	1.41	1.36
14	A3	835	CLA	C3C-C2C	2.22	1.41	1.36
16	F4	203	BCR	C30-C25	2.22	1.56	1.53
14	B4	805	CLA	O2A-CGA	2.22	1.39	1.33
14	A6	1641	CLA	C3C-C2C	2.23	1.41	1.36
14	B5	1805	CLA	C4C-C3C	2.23	1.48	1.45
14	B3	1809	CLA	C3C-C2C	2.23	1.41	1.36
14	B6	810	CLA	C3D-C2D	2.23	1.44	1.39
14	B1	827	CLA	O2A-CGA	2.23	1.39	1.33
14	B6	805	CLA	O2A-CGA	2.23	1.39	1.33
14	A2	1616	CLA	C3C-C2C	2.23	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B2	831	CLA	O2A-CGA	2.23	1.39	1.33
14	L5	206	CLA	O2D-CGD	2.23	1.38	1.33
14	A2	1607	CLA	C3D-C2D	2.23	1.44	1.39
14	L3	203	CLA	C3D-C2D	2.23	1.44	1.39
14	J5	101	CLA	C3D-C2D	2.23	1.44	1.39
14	A4	831	CLA	OBD-CAD	2.23	1.25	1.22
14	A6	1636	CLA	O2D-CGD	2.23	1.38	1.33
14	A6	1626	CLA	C3C-C2C	2.23	1.41	1.36
14	B4	820	CLA	C3D-C2D	2.23	1.44	1.39
14	X6	1701	CLA	C3C-C2C	2.23	1.41	1.36
14	B5	1831	CLA	C3D-C2D	2.23	1.44	1.39
14	L1	206	CLA	C3C-C2C	2.23	1.41	1.36
14	B2	840	CLA	O2D-CGD	2.23	1.38	1.33
14	B3	1835	CLA	C3D-C2D	2.23	1.44	1.39
14	B3	1835	CLA	C3C-C2C	2.23	1.41	1.36
14	L3	202	CLA	C3D-C2D	2.23	1.44	1.39
14	B4	831	CLA	C3C-C2C	2.23	1.41	1.36
14	B4	842	CLA	C3C-C2C	2.23	1.41	1.36
14	B5	1831	CLA	C3C-C2C	2.23	1.41	1.36
14	A5	838	CLA	C3D-C2D	2.23	1.44	1.39
14	B2	806	CLA	O2A-CGA	2.23	1.39	1.33
14	B1	809	CLA	O2A-CGA	2.23	1.39	1.33
14	B5	1808	CLA	C3C-C2C	2.23	1.41	1.36
14	A2	1644	CLA	O2D-CGD	2.23	1.38	1.33
14	B3	1836	CLA	O2D-CGD	2.23	1.38	1.33
14	A5	810	CLA	C3C-C2C	2.23	1.41	1.36
14	A4	828	CLA	O2A-CGA	2.23	1.39	1.33
16	A5	850	BCR	C30-C25	2.23	1.56	1.53
14	A5	805	CLA	C3C-C2C	2.23	1.41	1.36
14	A1	809	CLA	C3C-C2C	2.23	1.41	1.36
14	A5	828	CLA	C3C-C2C	2.23	1.41	1.36
14	M3	1601	CLA	C3D-C2D	2.23	1.44	1.39
14	A5	832	CLA	C3C-C2C	2.24	1.41	1.36
14	B6	813	CLA	O2A-CGA	2.24	1.39	1.33
14	B6	837	CLA	O2D-CGD	2.24	1.38	1.33
14	A4	822	CLA	C3C-C2C	2.24	1.41	1.36
14	I1	101	CLA	O2D-CGD	2.24	1.38	1.33
14	A4	826	CLA	C3D-C2D	2.24	1.44	1.39
14	B2	806	CLA	C3C-C2C	2.24	1.41	1.36
14	B4	804	CLA	O2D-CGD	2.24	1.38	1.33
14	B1	806	CLA	C4C-C3C	2.24	1.48	1.45
14	B6	836	CLA	C3C-C2C	2.24	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L3	205	CLA	O2D-CGD	2.24	1.38	1.33
14	B1	837	CLA	C3C-C2C	2.24	1.41	1.36
14	B1	827	CLA	C3B-C2B	2.24	1.43	1.40
14	B2	826	CLA	C3D-C2D	2.24	1.44	1.39
16	B1	852	BCR	C1-C6	2.24	1.56	1.53
14	B3	1808	CLA	O2A-CGA	2.24	1.39	1.33
14	B5	1838	CLA	C3C-C2C	2.24	1.41	1.36
14	A3	830	CLA	O2A-CGA	2.24	1.39	1.33
14	B6	810	CLA	O2D-CGD	2.24	1.38	1.33
14	L6	208	CLA	O2D-CGD	2.24	1.38	1.33
14	A6	1633	CLA	CHB-C4A	2.24	1.36	1.33
14	A6	1605	CLA	C3D-C2D	2.24	1.44	1.39
14	A5	838	CLA	C3C-C2C	2.24	1.41	1.36
14	A4	815	CLA	C3D-C2D	2.24	1.44	1.39
14	L5	202	CLA	C3D-C2D	2.24	1.44	1.39
14	A3	814	CLA	C3C-C2C	2.24	1.41	1.36
14	B4	811	CLA	O2A-CGA	2.24	1.39	1.33
14	A2	1609	CLA	C3C-C2C	2.24	1.41	1.36
14	L6	208	CLA	O2A-CGA	2.24	1.39	1.33
14	B6	817	CLA	C3D-C2D	2.24	1.44	1.39
14	B3	1831	CLA	C3D-C2D	2.24	1.44	1.39
14	B2	825	CLA	O2A-CGA	2.24	1.39	1.33
16	B4	846	BCR	C30-C25	2.24	1.56	1.53
14	A4	832	CLA	C3C-C2C	2.24	1.41	1.36
14	L4	204	CLA	O2D-CGD	2.25	1.38	1.33
14	K6	1401	CLA	C3C-C2C	2.25	1.41	1.36
14	A2	1631	CLA	O2A-CGA	2.25	1.39	1.33
14	A2	1605	CLA	C3D-C2D	2.25	1.44	1.39
14	A1	804	CLA	C3C-C2C	2.25	1.41	1.36
14	B6	823	CLA	C3C-C2C	2.25	1.41	1.36
14	B5	1805	CLA	O2A-CGA	2.25	1.39	1.33
14	B1	815	CLA	O2A-CGA	2.25	1.39	1.33
14	B4	831	CLA	C3D-C2D	2.25	1.44	1.39
14	B3	1812	CLA	C3D-C2D	2.25	1.44	1.39
14	B6	808	CLA	C3C-C2C	2.25	1.41	1.36
14	A5	835	CLA	C3C-C2C	2.25	1.41	1.36
14	A2	1632	CLA	C3C-C2C	2.25	1.41	1.36
16	A4	849	BCR	C30-C25	2.25	1.56	1.53
14	B4	829	CLA	C3D-C2D	2.25	1.44	1.39
14	B3	1827	CLA	C3D-C2D	2.25	1.44	1.39
14	A3	811	CLA	C3D-C2D	2.25	1.44	1.39
14	A4	802	CLA	C3D-C2D	2.25	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	802	CLA	O2A-CGA	2.25	1.39	1.33
16	B4	846	BCR	C8-C9	2.25	1.50	1.45
14	B3	1843	CLA	O2D-CGD	2.25	1.38	1.33
14	A2	1627	CLA	C3D-C2D	2.25	1.44	1.39
14	B3	1833	CLA	C3C-C2C	2.25	1.41	1.36
14	A1	828	CLA	O2A-CGA	2.25	1.39	1.33
14	B3	1826	CLA	C1C-C2C	2.25	1.48	1.44
14	B2	818	CLA	C3C-C2C	2.25	1.41	1.36
16	B5	1847	BCR	C1-C6	2.25	1.56	1.53
14	A2	1630	CLA	CHB-C4A	2.25	1.36	1.33
14	A2	1632	CLA	O2D-CGD	2.25	1.38	1.33
14	B3	1819	CLA	C3D-C2D	2.25	1.44	1.39
14	B1	834	CLA	C3D-C2D	2.25	1.44	1.39
14	B5	1804	CLA	OBD-CAD	2.25	1.25	1.22
14	B1	804	CLA	C1C-C2C	2.25	1.48	1.44
14	A2	1626	CLA	O2A-CGA	2.25	1.39	1.33
14	A6	1629	CLA	O2A-CGA	2.25	1.39	1.33
14	B1	804	CLA	C3C-C2C	2.26	1.41	1.36
14	A6	1620	CLA	C3D-C2D	2.26	1.44	1.39
14	B4	831	CLA	O2A-CGA	2.26	1.39	1.33
14	A3	820	CLA	C3D-C2D	2.26	1.44	1.39
14	A4	807	CLA	C1C-C2C	2.26	1.48	1.44
14	B4	828	CLA	O2A-CGA	2.26	1.39	1.33
14	A1	808	CLA	O2D-CGD	2.26	1.38	1.33
16	B3	1851	BCR	C1-C6	2.26	1.56	1.53
14	A2	1642	CLA	C3D-C2D	2.26	1.44	1.39
14	B3	1819	CLA	O2A-CGA	2.26	1.39	1.33
14	L5	205	CLA	O2D-CGD	2.26	1.38	1.33
14	A6	1630	CLA	C3C-C2C	2.26	1.41	1.36
14	L5	205	CLA	C3D-C2D	2.26	1.44	1.39
14	A2	1628	CLA	O2A-CGA	2.26	1.39	1.33
14	B3	1805	CLA	C4C-C3C	2.26	1.48	1.45
14	B5	1825	CLA	C3C-C2C	2.26	1.41	1.36
14	B2	833	CLA	O2D-CGD	2.26	1.38	1.33
14	B1	825	CLA	C1C-C2C	2.26	1.48	1.44
14	B1	854	CLA	O2D-CGD	2.26	1.38	1.33
14	B6	825	CLA	C3D-C2D	2.26	1.44	1.39
14	B1	835	CLA	O2D-CGD	2.26	1.38	1.33
14	A5	831	CLA	C3D-C2D	2.26	1.44	1.39
14	A5	834	CLA	C3C-C2C	2.26	1.41	1.36
14	B3	1803	CLA	C1C-C2C	2.26	1.48	1.44
14	B6	841	CLA	O2D-CGD	2.26	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B5	1834	CLA	O2A-CGA	2.26	1.39	1.33
14	A1	836	CLA	O2A-CGA	2.26	1.39	1.33
14	B1	808	CLA	O2A-CGA	2.26	1.39	1.33
14	B6	817	CLA	C3C-C2C	2.26	1.41	1.36
14	B4	805	CLA	O2D-CGD	2.26	1.38	1.33
14	L5	204	CLA	C3D-C2D	2.26	1.44	1.39
14	A6	1630	CLA	O2D-CGD	2.26	1.38	1.33
14	A2	1618	CLA	C3D-C2D	2.26	1.44	1.39
14	L6	206	CLA	OBD-CAD	2.26	1.25	1.22
14	B5	1805	CLA	O2D-CGD	2.26	1.38	1.33
14	B1	832	CLA	C3C-C2C	2.26	1.41	1.36
14	B1	806	CLA	O2D-CGD	2.26	1.38	1.33
14	B2	802	CLA	C3C-C2C	2.26	1.41	1.36
14	B3	1817	CLA	C3D-C2D	2.27	1.44	1.39
14	B5	1827	CLA	C3D-C2D	2.27	1.44	1.39
14	A1	820	CLA	C3C-C2C	2.27	1.41	1.36
14	A2	1607	CLA	C3C-C2C	2.27	1.41	1.36
14	L3	204	CLA	C3C-C2C	2.27	1.41	1.36
14	A3	841	CLA	C3D-C2D	2.27	1.44	1.39
14	A1	817	CLA	C3D-C2D	2.27	1.44	1.39
14	B1	805	CLA	C3C-C2C	2.27	1.41	1.36
14	A2	1628	CLA	C3C-C2C	2.27	1.41	1.36
14	A2	1613	CLA	C3D-C2D	2.27	1.44	1.39
16	B2	843	BCR	C8-C9	2.27	1.50	1.45
14	L1	201	CLA	C3C-C2C	2.27	1.41	1.36
14	B6	832	CLA	O2A-CGA	2.27	1.39	1.33
14	A5	818	CLA	C3D-C2D	2.27	1.44	1.39
14	A1	831	CLA	C3C-C2C	2.27	1.41	1.36
14	L3	202	CLA	C3C-C2C	2.27	1.41	1.36
14	B4	843	CLA	O2D-CGD	2.27	1.38	1.33
16	A6	1648	BCR	C1-C6	2.27	1.56	1.53
14	A1	808	CLA	C3C-C2C	2.27	1.41	1.36
16	B5	1845	BCR	C1-C6	2.27	1.56	1.53
14	A5	829	CLA	O2A-CGA	2.27	1.39	1.33
14	A6	1624	CLA	O2A-CGA	2.27	1.39	1.33
14	B1	841	CLA	O2D-CGD	2.27	1.38	1.33
14	B1	818	CLA	C3D-C2D	2.27	1.44	1.39
14	B2	802	CLA	C1C-C2C	2.27	1.48	1.44
14	A2	1640	CLA	C3C-C2C	2.27	1.41	1.36
14	A6	1638	CLA	O2A-CGA	2.27	1.39	1.33
14	B5	1842	CLA	OBD-CAD	2.27	1.25	1.22
14	A1	825	CLA	O2A-CGA	2.27	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B6	844	BCR	C8-C9	2.27	1.50	1.45
16	A1	847	BCR	C1-C6	2.27	1.56	1.53
14	B5	1833	CLA	C3C-C2C	2.27	1.41	1.36
14	A4	853	CLA	C3C-C2C	2.27	1.41	1.36
14	A3	822	CLA	C3C-C2C	2.27	1.41	1.36
14	B4	804	CLA	C3C-C2C	2.27	1.41	1.36
14	B6	829	CLA	O2A-CGA	2.27	1.39	1.33
14	A2	1612	CLA	C3C-C2C	2.27	1.41	1.36
14	B3	1812	CLA	O2D-CGD	2.27	1.38	1.33
14	A2	1625	CLA	C3D-C2D	2.27	1.44	1.39
14	B3	1830	CLA	C3D-C2D	2.27	1.44	1.39
17	X4	101	LHG	O8-C23	2.27	1.44	1.33
14	B5	1813	CLA	C3D-C2D	2.27	1.44	1.39
14	B2	839	CLA	OBD-CAD	2.27	1.25	1.22
14	K1	1401	CLA	C3C-C2C	2.27	1.41	1.36
14	B6	834	CLA	O2D-CGD	2.27	1.38	1.33
14	B4	805	CLA	C1C-C2C	2.27	1.48	1.44
14	A2	1603	CLA	O2A-CGA	2.27	1.39	1.33
14	B3	1805	CLA	O2A-CGA	2.27	1.39	1.33
14	A4	808	CLA	C3C-C2C	2.27	1.41	1.36
14	B5	1803	CLA	O2A-CGA	2.27	1.39	1.33
14	B6	831	CLA	C3C-C2C	2.28	1.41	1.36
14	A3	816	CLA	C3D-C2D	2.28	1.44	1.39
14	A3	810	CLA	C3C-C2C	2.28	1.41	1.36
14	B3	1828	CLA	O2A-CGA	2.28	1.39	1.33
17	B1	851	LHG	O8-C23	2.28	1.44	1.33
14	M6	1201	CLA	C3D-C2D	2.28	1.44	1.39
14	A5	824	CLA	O2A-CGA	2.28	1.39	1.33
14	B5	1827	CLA	O2A-CGA	2.28	1.40	1.32
14	A6	1651	CLA	C3C-C2C	2.28	1.41	1.36
16	A4	848	BCR	C1-C6	2.28	1.56	1.53
14	B5	1834	CLA	O2D-CGD	2.28	1.38	1.33
14	B1	833	CLA	O2D-CGD	2.28	1.38	1.33
14	B1	808	CLA	C3D-C2D	2.28	1.44	1.39
14	B5	1812	CLA	C3D-C2D	2.28	1.44	1.39
14	B2	803	CLA	C4C-C3C	2.28	1.49	1.45
16	J5	105	BCR	C1-C6	2.28	1.56	1.53
14	A6	1634	CLA	C3D-C2D	2.28	1.44	1.39
14	B3	1834	CLA	O2D-CGD	2.28	1.38	1.33
14	B2	805	CLA	O2A-CGA	2.28	1.39	1.33
14	A2	1617	CLA	C3C-C2C	2.28	1.41	1.36
14	A4	837	CLA	O2A-CGA	2.28	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A6	1626	CLA	O2A-CGA	2.28	1.39	1.33
14	A2	1638	CLA	O2D-CGD	2.28	1.38	1.33
14	B2	839	CLA	C3C-C2C	2.28	1.41	1.36
14	A5	811	CLA	C3D-C2D	2.28	1.44	1.39
14	A3	824	CLA	O2A-CGA	2.28	1.39	1.33
14	B3	1808	CLA	C3C-C2C	2.28	1.41	1.36
14	A6	1621	CLA	C3C-C2C	2.28	1.41	1.36
14	B2	826	CLA	O2D-CGD	2.28	1.38	1.33
14	A6	1621	CLA	C3D-C2D	2.28	1.44	1.39
16	A2	1649	BCR	C30-C25	2.28	1.56	1.53
14	L2	206	CLA	C3C-C2C	2.28	1.41	1.36
14	L5	202	CLA	C3C-C2C	2.29	1.41	1.36
14	A2	1610	CLA	C1C-C2C	2.29	1.49	1.44
14	B3	1838	CLA	C3C-C2C	2.29	1.41	1.36
14	B1	813	CLA	C3C-C2C	2.29	1.41	1.36
14	A5	821	CLA	C3C-C2C	2.29	1.41	1.36
14	J5	102	CLA	C3C-C2C	2.29	1.41	1.36
14	A6	1618	CLA	C3D-C2D	2.29	1.44	1.39
14	L4	201	CLA	CHB-C4A	2.29	1.36	1.33
16	B4	845	BCR	C1-C6	2.29	1.56	1.53
14	K4	1401	CLA	C3C-C2C	2.29	1.41	1.36
14	B5	1801	CLA	C3C-C2C	2.29	1.41	1.36
14	A3	802	CLA	O2A-CGA	2.29	1.39	1.33
14	B2	830	CLA	C3C-C2C	2.29	1.41	1.36
14	B4	819	CLA	C3C-C2C	2.29	1.41	1.36
14	L1	202	CLA	C3D-C2D	2.29	1.44	1.39
14	B4	840	CLA	C3D-C2D	2.29	1.44	1.39
14	B5	1836	CLA	O2D-CGD	2.29	1.38	1.33
16	B5	1846	BCR	C8-C9	2.29	1.50	1.45
14	B3	1816	CLA	C3C-C2C	2.29	1.41	1.36
14	L6	207	CLA	C3C-C2C	2.29	1.41	1.36
14	A1	810	CLA	C3D-C2D	2.29	1.44	1.39
16	A5	846	BCR	C30-C25	2.29	1.56	1.53
14	B6	803	CLA	O2A-CGA	2.29	1.40	1.33
14	A2	1620	CLA	C3D-C2D	2.29	1.44	1.39
14	A1	830	CLA	C3D-C2D	2.29	1.44	1.39
14	B6	802	CLA	OBD-CAD	2.29	1.25	1.22
14	B2	813	CLA	C3C-C2C	2.29	1.41	1.36
14	B2	801	CLA	O2A-CGA	2.29	1.40	1.33
14	A6	1620	CLA	O2D-CGD	2.29	1.38	1.33
14	B1	822	CLA	OBD-CAD	2.29	1.25	1.22
14	A1	822	CLA	C3D-C2D	2.29	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B6	849	LHG	O8-C23	2.29	1.44	1.33
17	X5	102	LHG	O8-C23	2.30	1.44	1.33
14	B1	841	CLA	O2A-CGA	2.30	1.40	1.33
14	B1	812	CLA	C3D-C2D	2.30	1.44	1.39
14	B6	830	CLA	C3D-C2D	2.30	1.44	1.39
14	A4	827	CLA	CHB-C4A	2.30	1.36	1.33
14	B1	808	CLA	C3C-C2C	2.30	1.41	1.36
14	B3	1805	CLA	C1C-C2C	2.30	1.49	1.44
14	A6	1609	CLA	O2A-CGA	2.30	1.40	1.33
14	A5	820	CLA	C3D-C2D	2.30	1.44	1.39
14	B2	808	CLA	C3D-C2D	2.30	1.44	1.39
14	B5	1811	CLA	C3D-C2D	2.30	1.44	1.39
14	A1	825	CLA	C3C-C2C	2.30	1.41	1.36
14	A3	815	CLA	C3C-C2C	2.30	1.41	1.36
14	X2	1701	CLA	O2D-CGD	2.30	1.39	1.33
14	B5	1843	CLA	O2D-CGD	2.30	1.39	1.33
14	A1	827	CLA	C3C-C2C	2.30	1.41	1.36
14	A5	837	CLA	O2A-CGA	2.30	1.40	1.33
14	A5	826	CLA	O2A-CGA	2.30	1.40	1.33
14	J4	101	CLA	C3D-C2D	2.30	1.44	1.39
14	B4	808	CLA	O2A-CGA	2.30	1.40	1.33
14	B4	837	CLA	C3D-C2D	2.30	1.44	1.39
16	M1	1202	BCR	C1-C6	2.30	1.56	1.53
14	J6	1103	CLA	C3C-C2C	2.30	1.41	1.36
14	A1	822	CLA	C3C-C2C	2.30	1.41	1.36
14	B4	834	CLA	C3D-C2D	2.30	1.44	1.39
14	B4	828	CLA	C3B-C2B	2.30	1.43	1.40
14	A5	838	CLA	O2A-CGA	2.30	1.40	1.33
14	A1	820	CLA	C3D-C2D	2.30	1.44	1.39
16	B1	845	BCR	C1-C6	2.30	1.56	1.53
14	B2	816	CLA	C3D-C2D	2.30	1.44	1.39
14	A1	815	CLA	C3D-C2D	2.30	1.44	1.39
14	A4	829	CLA	C3C-C2C	2.30	1.41	1.36
14	A4	825	CLA	C3C-C2C	2.30	1.41	1.36
14	A5	809	CLA	O2A-CGA	2.30	1.40	1.33
14	B5	1828	CLA	O2A-CGA	2.30	1.40	1.33
14	B3	1803	CLA	O2A-CGA	2.30	1.40	1.33
16	A5	847	BCR	C1-C6	2.30	1.56	1.53
14	A3	825	CLA	C3C-C2C	2.30	1.41	1.36
14	A6	1625	CLA	C3C-C2C	2.30	1.41	1.36
14	B2	804	CLA	O2A-CGA	2.30	1.40	1.33
14	B6	829	CLA	C3D-C2D	2.30	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A6	1603	CLA	C3D-C2D	2.30	1.44	1.39
14	L4	204	CLA	C3C-C2C	2.30	1.41	1.36
14	B3	1804	CLA	OBD-CAD	2.31	1.25	1.22
16	F4	204	BCR	C1-C6	2.31	1.56	1.53
14	B4	826	CLA	C1C-C2C	2.31	1.49	1.44
14	B5	1802	CLA	C3D-C2D	2.31	1.44	1.39
14	B6	811	CLA	C3D-C2D	2.31	1.44	1.39
14	L3	204	CLA	O2D-CGD	2.31	1.39	1.33
14	J1	101	CLA	C1C-C2C	2.31	1.49	1.44
14	B3	1811	CLA	C3D-C2D	2.31	1.44	1.39
14	B1	801	CLA	O2A-CGA	2.31	1.40	1.33
16	A2	1648	BCR	C30-C25	2.31	1.56	1.53
14	B3	1802	CLA	C3D-C2D	2.31	1.44	1.39
14	A6	1601	CLA	C3D-C2D	2.31	1.44	1.39
14	B4	802	CLA	C3D-C2D	2.31	1.44	1.39
14	A4	820	CLA	C3C-C2C	2.31	1.41	1.36
14	A6	1611	CLA	C3D-C2D	2.31	1.44	1.39
14	A5	816	CLA	O2A-CGA	2.31	1.40	1.33
14	B1	807	CLA	O2A-CGA	2.31	1.40	1.33
14	B2	824	CLA	C3D-C2D	2.31	1.44	1.39
14	I6	101	CLA	OBD-CAD	2.31	1.25	1.22
14	B6	832	CLA	O2D-CGD	2.31	1.39	1.33
14	L2	205	CLA	C3D-C2D	2.31	1.44	1.39
14	B5	1826	CLA	C1C-C2C	2.31	1.49	1.44
14	B1	834	CLA	C3C-C2C	2.31	1.41	1.36
14	B2	801	CLA	O2D-CGD	2.31	1.39	1.33
14	A3	826	CLA	O2A-CGA	2.31	1.40	1.33
14	B4	833	CLA	C3C-C2C	2.31	1.41	1.36
14	B2	805	CLA	C3D-C2D	2.31	1.44	1.39
14	B2	811	CLA	C3C-C2C	2.31	1.41	1.36
14	A4	813	CLA	C3C-C2C	2.31	1.41	1.36
14	L4	201	CLA	C3D-C2D	2.31	1.44	1.39
14	A5	821	CLA	C3D-C2D	2.31	1.44	1.39
16	B3	1846	BCR	C8-C9	2.31	1.50	1.45
14	B3	1814	CLA	C3C-C2C	2.31	1.41	1.36
14	L6	203	CLA	C3D-C2D	2.31	1.44	1.39
14	B1	810	CLA	O2A-CGA	2.32	1.40	1.33
14	J6	1101	CLA	C3D-C2D	2.32	1.44	1.39
14	B4	843	CLA	O2A-CGA	2.32	1.40	1.33
14	B2	807	CLA	O2A-CGA	2.32	1.40	1.33
17	A6	1649	LHG	P-O6	2.32	1.68	1.59
14	A5	839	CLA	O2A-CGA	2.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B2	849	LHG	O8-C23	2.32	1.44	1.33
17	X3	101	LHG	O8-C23	2.32	1.44	1.33
14	B6	840	CLA	C3C-C2C	2.32	1.41	1.36
14	B3	1843	CLA	O2A-CGA	2.32	1.40	1.33
14	A6	1621	CLA	O2A-CGA	2.32	1.40	1.33
14	X6	1701	CLA	O2D-CGD	2.32	1.39	1.33
14	A3	839	CLA	O2A-CGA	2.32	1.40	1.33
14	A3	809	CLA	O2A-CGA	2.32	1.40	1.33
14	A6	1614	CLA	C3C-C2C	2.32	1.41	1.36
14	B4	801	CLA	OBD-CAD	2.32	1.25	1.22
14	B5	1839	CLA	O2D-CGD	2.32	1.39	1.33
14	B6	819	CLA	O2D-CGD	2.32	1.39	1.33
14	B5	1804	CLA	C3C-C2C	2.32	1.41	1.36
14	A3	830	CLA	C3C-C2C	2.32	1.41	1.36
14	B4	837	CLA	C3C-C2C	2.32	1.41	1.36
14	X3	102	CLA	O2D-CGD	2.32	1.39	1.33
14	A2	1622	CLA	O2D-CGD	2.32	1.39	1.33
14	B6	809	CLA	C3D-C2D	2.32	1.44	1.39
14	B3	1834	CLA	O2A-CGA	2.32	1.40	1.33
14	L1	206	CLA	O2D-CGD	2.32	1.39	1.33
14	B1	838	CLA	O2D-CGD	2.32	1.39	1.33
14	B4	834	CLA	O2A-CGA	2.32	1.40	1.33
14	A3	830	CLA	C3D-C2D	2.32	1.44	1.39
14	B4	825	CLA	C3C-C2C	2.32	1.41	1.36
14	B4	817	CLA	O2D-CGD	2.32	1.39	1.33
14	M3	1601	CLA	C3C-C2C	2.32	1.41	1.36
14	A5	815	CLA	C3C-C2C	2.32	1.41	1.36
14	B2	802	CLA	O2A-CGA	2.32	1.40	1.33
16	B1	844	BCR	C8-C9	2.32	1.51	1.45
14	A6	1615	CLA	C3C-C2C	2.32	1.41	1.36
14	B3	1810	CLA	O2D-CGD	2.32	1.39	1.33
14	B1	811	CLA	C3D-C2D	2.32	1.44	1.39
14	B1	806	CLA	C1C-C2C	2.32	1.49	1.44
14	A3	820	CLA	C3C-C2C	2.32	1.41	1.36
14	B4	819	CLA	C3D-C2D	2.32	1.44	1.39
14	B3	1829	CLA	O2D-CGD	2.33	1.39	1.33
14	A3	830	CLA	O2D-CGD	2.33	1.39	1.33
14	A4	835	CLA	O2D-CGD	2.33	1.39	1.33
14	A3	824	CLA	C3C-C2C	2.33	1.41	1.36
14	B4	804	CLA	O2A-CGA	2.33	1.40	1.33
14	A3	824	CLA	O2D-CGD	2.33	1.39	1.33
14	A5	813	CLA	C3D-C2D	2.33	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A3	835	CLA	O2A-CGA	2.33	1.40	1.33
14	B5	1806	CLA	OBD-CAD	2.33	1.25	1.22
14	A4	829	CLA	O2D-CGD	2.33	1.39	1.33
14	B6	804	CLA	O2A-CGA	2.33	1.40	1.33
14	B4	842	CLA	OBD-CAD	2.33	1.25	1.22
14	A6	1651	CLA	OBD-CAD	2.33	1.25	1.22
14	A4	823	CLA	O2A-CGA	2.33	1.40	1.33
14	A2	1623	CLA	C3C-C2C	2.33	1.41	1.36
14	A6	1633	CLA	C3D-C2D	2.33	1.44	1.39
14	B2	821	CLA	C3C-C2C	2.33	1.41	1.36
14	B3	1828	CLA	C3B-C2B	2.33	1.43	1.40
14	A1	805	CLA	C3D-C2D	2.33	1.44	1.39
14	B2	835	CLA	C3D-C2D	2.33	1.44	1.39
14	A3	834	CLA	C3D-C2D	2.33	1.44	1.39
14	A4	824	CLA	C3D-C2D	2.33	1.44	1.39
14	B2	803	CLA	O2D-CGD	2.33	1.39	1.33
14	A1	829	CLA	C3C-C2C	2.33	1.41	1.36
14	A3	818	CLA	C3D-C2D	2.33	1.44	1.39
14	A4	810	CLA	C3D-C2D	2.33	1.44	1.39
14	A4	808	CLA	O2D-CGD	2.33	1.39	1.33
14	B6	802	CLA	O2A-CGA	2.33	1.40	1.33
14	B2	819	CLA	C3C-C2C	2.33	1.41	1.36
14	B5	1804	CLA	O2A-CGA	2.33	1.40	1.33
14	A5	824	CLA	C3C-C2C	2.33	1.41	1.36
14	B4	808	CLA	C3C-C2C	2.33	1.41	1.36
14	B3	1842	CLA	OBD-CAD	2.33	1.25	1.22
14	L2	202	CLA	C3D-C2D	2.33	1.44	1.39
14	B2	810	CLA	C3D-C2D	2.33	1.44	1.39
14	B5	1814	CLA	C3C-C2C	2.34	1.41	1.36
14	J1	102	CLA	C3C-C2C	2.34	1.41	1.36
14	B6	814	CLA	C3C-C2C	2.34	1.41	1.36
14	B3	1828	CLA	C3D-C2D	2.34	1.44	1.39
14	A2	1634	CLA	OBD-CAD	2.34	1.25	1.22
14	B6	812	CLA	C3C-C2C	2.34	1.41	1.36
14	L4	205	CLA	O2A-CGA	2.34	1.40	1.33
14	A5	816	CLA	C3D-C2D	2.34	1.44	1.39
14	B5	1807	CLA	O2A-CGA	2.34	1.40	1.33
14	L5	203	CLA	CHB-C4A	2.34	1.36	1.33
14	B4	832	CLA	C3D-C2D	2.34	1.44	1.39
14	A1	832	CLA	C3D-C2D	2.34	1.44	1.39
14	B2	816	CLA	C3C-C2C	2.34	1.41	1.36
14	A4	820	CLA	C3D-C2D	2.34	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A1	818	CLA	CHB-C4A	2.34	1.36	1.33
14	A3	821	CLA	OBD-CAD	2.34	1.25	1.22
14	A1	802	CLA	C3D-C2D	2.34	1.44	1.39
14	B4	827	CLA	O2D-CGD	2.34	1.39	1.33
14	B2	824	CLA	O2D-CGD	2.34	1.39	1.33
17	A3	853	LHG	P-O6	2.34	1.68	1.59
14	B1	826	CLA	C3D-C2D	2.34	1.44	1.39
14	B4	825	CLA	C3D-C2D	2.34	1.44	1.39
14	A2	1626	CLA	O2D-CGD	2.34	1.39	1.33
14	A4	838	CLA	O2A-CGA	2.34	1.40	1.33
14	A4	804	CLA	C3C-C2C	2.34	1.41	1.36
14	L5	203	CLA	C3D-C2D	2.34	1.44	1.39
14	B4	825	CLA	O2D-CGD	2.34	1.39	1.33
14	B3	1817	CLA	O2D-CGD	2.34	1.39	1.33
14	F2	204	CLA	C3C-C2C	2.35	1.41	1.36
14	B4	834	CLA	O2D-CGD	2.35	1.39	1.33
14	A2	1611	CLA	O2A-CGA	2.35	1.40	1.33
14	B3	1819	CLA	C3C-C2C	2.35	1.41	1.36
14	A2	1624	CLA	C3C-C2C	2.35	1.41	1.36
14	A2	1627	CLA	C3C-C2C	2.35	1.41	1.36
14	M6	1201	CLA	OBD-CAD	2.35	1.25	1.22
14	L1	207	CLA	O2A-CGA	2.35	1.40	1.33
14	X1	1701	CLA	O2D-CGD	2.35	1.39	1.33
14	B4	809	CLA	C3C-C2C	2.35	1.41	1.36
14	A6	1606	CLA	C3D-C2D	2.35	1.44	1.39
14	L1	205	CLA	C3D-C2D	2.35	1.44	1.39
14	L4	204	CLA	C3D-C2D	2.35	1.44	1.39
14	A1	812	CLA	O2A-CGA	2.35	1.40	1.33
14	B2	818	CLA	C3D-C2D	2.35	1.44	1.39
14	B6	806	CLA	O2A-CGA	2.35	1.40	1.33
14	A6	1616	CLA	O2A-CGA	2.35	1.40	1.33
14	A5	839	CLA	C3C-C2C	2.35	1.41	1.36
14	L6	207	CLA	O2D-CGD	2.35	1.39	1.33
14	X5	101	CLA	O2D-CGD	2.35	1.39	1.33
14	A2	1628	CLA	OBD-CAD	2.35	1.25	1.22
14	L1	206	CLA	C3D-C2D	2.35	1.44	1.39
14	B3	1823	CLA	C3C-C2C	2.35	1.41	1.36
14	A5	834	CLA	O2A-CGA	2.35	1.40	1.33
14	A4	825	CLA	O2A-CGA	2.35	1.40	1.33
14	B2	824	CLA	O2A-CGA	2.35	1.40	1.32
14	A3	821	CLA	C3C-C2C	2.35	1.41	1.36
14	A4	833	CLA	O2A-CGA	2.36	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B2	829	CLA	C3D-C2D	2.36	1.44	1.39
14	B4	811	CLA	C3D-C2D	2.36	1.44	1.39
14	A6	1609	CLA	O2D-CGD	2.36	1.39	1.33
14	B1	826	CLA	O2A-CGA	2.36	1.40	1.32
14	B4	810	CLA	O2A-CGA	2.36	1.40	1.33
14	A6	1624	CLA	C3C-C2C	2.36	1.41	1.36
14	A5	813	CLA	O2A-CGA	2.36	1.40	1.33
14	A5	830	CLA	C3C-C2C	2.36	1.41	1.36
14	A5	822	CLA	C3C-C2C	2.36	1.41	1.36
14	A2	1644	CLA	C3D-C2D	2.36	1.44	1.39
14	A5	824	CLA	O2D-CGD	2.36	1.39	1.33
14	A5	819	CLA	O2A-CGA	2.36	1.40	1.33
14	L3	205	CLA	O2A-CGA	2.36	1.40	1.33
14	L1	202	CLA	CHB-C4A	2.36	1.36	1.33
14	A4	809	CLA	C3C-C2C	2.36	1.41	1.36
14	A3	839	CLA	C3D-C2D	2.36	1.44	1.39
14	B1	833	CLA	O2A-CGA	2.36	1.40	1.33
14	A6	1601	CLA	C3C-C2C	2.36	1.41	1.36
14	B3	1827	CLA	O2D-CGD	2.36	1.39	1.33
14	B1	828	CLA	O2D-CGD	2.36	1.39	1.33
14	B4	803	CLA	C1C-C2C	2.36	1.49	1.44
14	B1	805	CLA	OBD-CAD	2.36	1.25	1.22
14	A5	842	CLA	C3D-C2D	2.36	1.44	1.39
14	B5	1829	CLA	O2D-CGD	2.36	1.39	1.33
14	B2	828	CLA	C3D-C2D	2.36	1.44	1.39
14	B6	836	CLA	C3D-C2D	2.36	1.44	1.39
14	B1	820	CLA	C3C-C2C	2.36	1.41	1.36
14	A1	824	CLA	C3D-C2D	2.36	1.44	1.39
14	B5	1810	CLA	O2A-CGA	2.37	1.40	1.33
14	B2	819	CLA	C3D-C2D	2.37	1.44	1.39
14	L2	207	CLA	O2A-CGA	2.37	1.40	1.33
14	A1	813	CLA	C3C-C2C	2.37	1.41	1.36
14	B1	808	CLA	OBD-CAD	2.37	1.25	1.22
14	A5	840	CLA	C3D-C2D	2.37	1.44	1.39
14	A5	837	CLA	C3D-C2D	2.37	1.44	1.39
14	B6	822	CLA	C3C-C2C	2.37	1.41	1.36
14	B4	822	CLA	C3D-C2D	2.37	1.44	1.39
14	A6	1634	CLA	O2A-CGA	2.37	1.40	1.33
14	B6	835	CLA	C3C-C2C	2.37	1.41	1.36
14	A1	834	CLA	C3D-C2D	2.37	1.44	1.39
14	B2	809	CLA	C3D-C2D	2.37	1.44	1.39
14	J4	102	CLA	C3C-C2C	2.37	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B6	825	CLA	O2A-CGA	2.37	1.40	1.32
14	B6	819	CLA	C3D-C2D	2.37	1.44	1.39
14	B3	1841	CLA	O2D-CGD	2.37	1.39	1.33
14	A2	1618	CLA	O2A-CGA	2.37	1.40	1.33
14	B5	1805	CLA	C3D-C2D	2.37	1.44	1.39
14	B1	836	CLA	C3C-C2C	2.37	1.41	1.36
14	B4	829	CLA	O2D-CGD	2.37	1.39	1.33
14	A6	1622	CLA	C3C-C2C	2.37	1.41	1.36
14	B6	826	CLA	O2A-CGA	2.37	1.40	1.33
14	B5	1810	CLA	O2D-CGD	2.37	1.39	1.33
14	B1	805	CLA	O2A-CGA	2.37	1.40	1.33
14	B6	802	CLA	C3C-C2C	2.37	1.41	1.36
14	B4	805	CLA	C3D-C2D	2.37	1.44	1.39
14	B6	838	CLA	C3D-C2D	2.37	1.44	1.39
14	B5	1840	CLA	C3D-C2D	2.37	1.44	1.39
14	B2	834	CLA	C3C-C2C	2.37	1.41	1.36
14	B6	804	CLA	O2D-CGD	2.37	1.39	1.33
14	L2	206	CLA	O2D-CGD	2.37	1.39	1.33
14	B3	1807	CLA	O2D-CGD	2.38	1.39	1.33
14	B1	801	CLA	C3C-C2C	2.38	1.41	1.36
14	A3	802	CLA	C3C-C2C	2.38	1.41	1.36
14	B4	812	CLA	C3D-C2D	2.38	1.44	1.39
14	A2	1623	CLA	O2A-CGA	2.38	1.40	1.33
14	A3	819	CLA	O2A-CGA	2.38	1.40	1.33
14	A4	836	CLA	O2A-CGA	2.38	1.40	1.33
14	A1	808	CLA	O2A-CGA	2.38	1.40	1.33
14	B3	1824	CLA	C3C-C2C	2.38	1.41	1.36
14	L6	202	CLA	OBD-CAD	2.38	1.25	1.22
14	A4	812	CLA	O2A-CGA	2.38	1.40	1.33
14	M2	1201	CLA	OBD-CAD	2.38	1.25	1.22
14	A5	820	CLA	O2D-CGD	2.38	1.39	1.33
14	K3	1401	CLA	C3D-C2D	2.38	1.44	1.39
14	A4	824	CLA	C3C-C2C	2.38	1.41	1.36
14	A5	802	CLA	C3C-C2C	2.38	1.41	1.36
14	A5	819	CLA	CHB-C4A	2.38	1.36	1.33
14	B4	804	CLA	OBD-CAD	2.38	1.25	1.22
14	B3	1837	CLA	C3D-C2D	2.38	1.44	1.39
14	B3	1810	CLA	O2A-CGA	2.38	1.40	1.33
14	B3	1821	CLA	C3D-C2D	2.38	1.44	1.39
14	A2	1637	CLA	C3D-C2D	2.38	1.44	1.39
14	B5	1821	CLA	C3C-C2C	2.38	1.41	1.36
14	A3	803	CLA	O2A-CGA	2.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	806	CLA	C3D-C2D	2.38	1.44	1.39
14	A4	821	CLA	C3C-C2C	2.38	1.41	1.36
14	A1	824	CLA	C3C-C2C	2.38	1.41	1.36
14	B5	1817	CLA	O2D-CGD	2.38	1.39	1.33
14	B2	803	CLA	C3D-C2D	2.38	1.44	1.39
14	A5	825	CLA	C3C-C2C	2.38	1.41	1.36
14	B3	1807	CLA	O2A-CGA	2.38	1.40	1.33
14	A2	1608	CLA	C3D-C2D	2.38	1.44	1.39
14	A5	820	CLA	C3C-C2C	2.39	1.41	1.36
14	A4	819	CLA	C3C-C2C	2.39	1.41	1.36
17	B6	849	LHG	P-O4	2.39	1.66	1.55
14	B5	1843	CLA	O2A-CGA	2.39	1.40	1.33
14	B2	804	CLA	O2D-CGD	2.39	1.39	1.33
14	B6	841	CLA	O2A-CGA	2.39	1.40	1.33
14	B5	1827	CLA	O2D-CGD	2.39	1.39	1.33
14	A1	835	CLA	O2A-CGA	2.39	1.40	1.33
14	A3	838	CLA	O2A-CGA	2.39	1.40	1.33
14	A2	1639	CLA	O2A-CGA	2.39	1.40	1.33
14	A4	808	CLA	O2A-CGA	2.39	1.40	1.33
14	A1	812	CLA	C3D-C2D	2.39	1.44	1.39
14	A3	825	CLA	C3D-C2D	2.39	1.44	1.39
14	B1	802	CLA	C3D-C2D	2.39	1.44	1.39
16	B1	843	BCR	C1-C6	2.39	1.57	1.53
14	B5	1821	CLA	O2A-CGA	2.39	1.40	1.33
14	B2	803	CLA	C1C-C2C	2.39	1.49	1.44
14	A1	823	CLA	O2D-CGD	2.39	1.39	1.33
14	B2	834	CLA	C3D-C2D	2.39	1.44	1.39
14	L3	203	CLA	OBD-CAD	2.39	1.25	1.22
14	L4	201	CLA	O2A-CGA	2.39	1.40	1.33
14	A1	819	CLA	C3C-C2C	2.39	1.41	1.36
14	A6	1626	CLA	OBD-CAD	2.39	1.25	1.22
14	B2	840	CLA	O2A-CGA	2.39	1.40	1.33
14	B4	803	CLA	O2A-CGA	2.39	1.40	1.33
14	A6	1620	CLA	C3C-C2C	2.39	1.41	1.36
14	B1	823	CLA	OBD-CAD	2.39	1.25	1.22
14	A6	1637	CLA	O2A-CGA	2.39	1.40	1.33
14	A4	812	CLA	C3D-C2D	2.39	1.44	1.39
14	L5	205	CLA	C3C-C2C	2.39	1.41	1.36
14	B6	807	CLA	C3C-C2C	2.39	1.41	1.36
14	B5	1803	CLA	O2D-CGD	2.39	1.39	1.33
14	B5	1807	CLA	C3D-C2D	2.39	1.44	1.39
14	A6	1638	CLA	C3D-C2D	2.39	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B6	835	CLA	C3D-C2D	2.39	1.44	1.39
14	B6	819	CLA	C3C-C2C	2.40	1.41	1.36
14	J3	102	CLA	C3C-C2C	2.40	1.41	1.36
14	B1	854	CLA	C3D-C2D	2.40	1.44	1.39
14	B3	1822	CLA	C3C-C2C	2.40	1.41	1.36
14	B2	818	CLA	O2A-CGA	2.40	1.40	1.33
14	B1	805	CLA	C1C-C2C	2.40	1.49	1.44
14	B1	820	CLA	O2A-CGA	2.40	1.40	1.33
14	B1	839	CLA	C3D-C2D	2.40	1.44	1.39
14	B4	824	CLA	C3C-C2C	2.40	1.41	1.36
14	A6	1603	CLA	O2D-CGD	2.40	1.39	1.33
14	A1	829	CLA	C3D-C2D	2.40	1.44	1.39
14	B1	820	CLA	C3D-C2D	2.40	1.44	1.39
14	A2	1621	CLA	O2A-CGA	2.40	1.40	1.33
14	A3	807	CLA	O2D-CGD	2.40	1.39	1.33
14	A3	822	CLA	C3D-C2D	2.40	1.44	1.39
14	A4	817	CLA	C3D-C2D	2.40	1.44	1.39
14	B4	816	CLA	C3C-C2C	2.40	1.41	1.36
14	A3	813	CLA	O2A-CGA	2.40	1.40	1.33
14	B1	818	CLA	CHB-C4A	2.40	1.36	1.33
14	B3	1826	CLA	C3C-C2C	2.40	1.41	1.36
14	A3	809	CLA	O2D-CGD	2.40	1.39	1.33
14	A1	805	CLA	O2A-CGA	2.40	1.40	1.33
14	A6	1651	CLA	C1C-C2C	2.40	1.49	1.44
14	B5	1825	CLA	O2D-CGD	2.40	1.39	1.33
14	B6	839	CLA	O2D-CGD	2.40	1.39	1.33
14	B3	1833	CLA	CHB-C4A	2.40	1.36	1.33
14	B2	802	CLA	OBD-CAD	2.40	1.25	1.22
14	B4	807	CLA	O2D-CGD	2.40	1.39	1.33
14	A4	831	CLA	O2D-CGD	2.40	1.39	1.33
14	A1	823	CLA	C3C-C2C	2.40	1.41	1.36
14	B5	1840	CLA	C3C-C2C	2.40	1.41	1.36
14	B4	806	CLA	OBD-CAD	2.40	1.25	1.22
14	B2	822	CLA	O2D-CGD	2.40	1.39	1.33
16	A6	1645	BCR	C1-C6	2.41	1.57	1.53
14	A4	815	CLA	O2A-CGA	2.41	1.40	1.33
14	B5	1802	CLA	O2D-CGD	2.41	1.39	1.33
14	B6	807	CLA	OBD-CAD	2.41	1.25	1.22
14	B4	838	CLA	C3D-C2D	2.41	1.44	1.39
14	A2	1626	CLA	C3C-C2C	2.41	1.41	1.36
14	A1	819	CLA	O2D-CGD	2.41	1.39	1.33
14	J3	101	CLA	C3C-C2C	2.41	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B4	826	CLA	CHB-C4A	2.41	1.36	1.33
14	B5	1826	CLA	CHB-C4A	2.41	1.36	1.33
14	B5	1816	CLA	C3C-C2C	2.41	1.41	1.36
14	B4	821	CLA	O2A-CGA	2.41	1.40	1.33
14	B5	1834	CLA	C3D-C2D	2.41	1.44	1.39
14	L5	206	CLA	O2A-CGA	2.41	1.40	1.33
14	B5	1801	CLA	O2A-CGA	2.41	1.40	1.33
14	A1	832	CLA	O2A-CGA	2.41	1.40	1.33
14	A4	818	CLA	O2A-CGA	2.41	1.40	1.33
14	A2	1622	CLA	C3C-C2C	2.41	1.41	1.36
14	B4	814	CLA	C3C-C2C	2.41	1.41	1.36
14	B5	1821	CLA	C3D-C2D	2.41	1.44	1.39
14	L4	203	CLA	C1C-C2C	2.41	1.49	1.44
14	B6	806	CLA	O2D-CGD	2.41	1.39	1.33
14	B3	1806	CLA	OBD-CAD	2.41	1.25	1.22
14	B4	824	CLA	C3D-C2D	2.41	1.44	1.39
14	B4	827	CLA	O2A-CGA	2.41	1.40	1.32
14	A3	820	CLA	O2D-CGD	2.41	1.39	1.33
14	B6	823	CLA	O2D-CGD	2.41	1.39	1.33
14	B2	810	CLA	C3C-C2C	2.41	1.41	1.36
14	A3	816	CLA	O2A-CGA	2.41	1.40	1.33
14	A6	1635	CLA	C3D-C2D	2.41	1.44	1.39
14	B4	807	CLA	O2A-CGA	2.42	1.40	1.33
14	B3	1821	CLA	O2A-CGA	2.42	1.40	1.33
14	A5	825	CLA	C3D-C2D	2.42	1.44	1.39
14	B5	1804	CLA	C1C-C2C	2.42	1.49	1.44
14	A3	840	CLA	C3C-C2C	2.42	1.41	1.36
14	A3	843	CLA	C3D-C2D	2.42	1.44	1.39
14	B3	1801	CLA	O2A-CGA	2.42	1.40	1.33
14	B3	1821	CLA	O2D-CGD	2.42	1.39	1.33
14	A2	1611	CLA	O2D-CGD	2.42	1.39	1.33
14	B3	1825	CLA	O2D-CGD	2.42	1.39	1.33
14	L3	205	CLA	C3D-C2D	2.42	1.44	1.39
14	B6	808	CLA	O2A-CGA	2.42	1.40	1.33
14	B3	1840	CLA	C3C-C2C	2.42	1.41	1.36
14	B2	804	CLA	C3D-C2D	2.42	1.44	1.39
14	A4	814	CLA	C3C-C2C	2.42	1.41	1.36
14	B3	1802	CLA	O2D-CGD	2.42	1.39	1.33
14	A2	1640	CLA	C3D-C2D	2.42	1.44	1.39
14	B2	814	CLA	O2D-CGD	2.42	1.39	1.33
14	B3	1827	CLA	O2A-CGA	2.42	1.40	1.32
14	A2	1641	CLA	C3C-C2C	2.42	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	806	CLA	O2A-CGA	2.42	1.40	1.33
14	B4	828	CLA	C3D-C2D	2.42	1.44	1.39
17	A2	1653	LHG	P-O6	2.42	1.69	1.59
14	B4	804	CLA	C1C-C2C	2.42	1.49	1.44
14	A6	1606	CLA	O2A-CGA	2.42	1.40	1.33
17	A3	854	LHG	P-O3	2.42	1.69	1.59
14	B3	1813	CLA	C3C-C2C	2.42	1.41	1.36
14	B1	815	CLA	C3C-C2C	2.42	1.41	1.36
17	A4	850	LHG	P-O6	2.43	1.69	1.59
14	B1	821	CLA	C3C-C2C	2.43	1.41	1.36
14	B5	1837	CLA	C3C-C2C	2.43	1.41	1.36
14	L4	203	CLA	C3D-C2D	2.43	1.44	1.39
14	A1	837	CLA	C3D-C2D	2.43	1.44	1.39
14	A6	1618	CLA	O2A-CGA	2.43	1.40	1.33
14	B2	837	CLA	C3D-C2D	2.43	1.44	1.39
14	A3	845	CLA	C3D-C2D	2.43	1.44	1.39
14	A5	830	CLA	C3D-C2D	2.43	1.44	1.39
14	A4	838	CLA	C3C-C2C	2.43	1.41	1.36
14	A5	823	CLA	O2D-CGD	2.43	1.39	1.33
14	A1	827	CLA	CHB-C4A	2.43	1.36	1.33
14	B1	827	CLA	C3D-C2D	2.43	1.44	1.39
14	A4	823	CLA	O2D-CGD	2.43	1.39	1.33
14	A6	1613	CLA	O2A-CGA	2.43	1.40	1.33
14	A2	1632	CLA	C3D-C2D	2.43	1.44	1.39
14	A5	843	CLA	C3D-C2D	2.43	1.44	1.39
14	A1	821	CLA	C3D-C2D	2.43	1.44	1.39
14	B5	1834	CLA	C3C-C2C	2.43	1.41	1.36
14	L4	203	CLA	OBD-CAD	2.43	1.25	1.22
14	A3	814	CLA	C3D-C2D	2.43	1.44	1.39
14	B5	1832	CLA	C3D-C2D	2.43	1.44	1.39
14	B5	1808	CLA	O2D-CGD	2.43	1.39	1.33
14	A2	1617	CLA	C3D-C2D	2.43	1.44	1.39
14	B6	821	CLA	C3C-C2C	2.43	1.41	1.36
14	B1	827	CLA	O2D-CGD	2.43	1.39	1.33
14	B3	1834	CLA	C3C-C2C	2.43	1.41	1.36
14	A3	813	CLA	C3D-C2D	2.43	1.44	1.39
14	B2	838	CLA	O2D-CGD	2.43	1.39	1.33
14	B2	816	CLA	CHB-C4A	2.43	1.36	1.33
14	B5	1808	CLA	OBD-CAD	2.43	1.25	1.22
14	B6	807	CLA	O2D-CGD	2.43	1.39	1.33
14	B1	839	CLA	O2A-CGA	2.43	1.40	1.33
14	B1	808	CLA	O2D-CGD	2.43	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J6	1102	CLA	C3C-C2C	2.43	1.41	1.36
14	B1	837	CLA	C3D-C2D	2.43	1.44	1.39
14	B6	805	CLA	C1C-C2C	2.43	1.49	1.44
14	B5	1841	CLA	O2D-CGD	2.43	1.39	1.33
14	B6	822	CLA	C3D-C2D	2.43	1.44	1.39
14	B3	1821	CLA	C3C-C2C	2.43	1.41	1.36
14	A1	820	CLA	O2A-CGA	2.44	1.40	1.33
14	A1	814	CLA	C3D-C2D	2.44	1.44	1.39
14	A3	845	CLA	O2A-CGA	2.44	1.40	1.33
17	X4	101	LHG	P-O4	2.44	1.67	1.55
14	B5	1807	CLA	O2D-CGD	2.44	1.39	1.33
14	B6	820	CLA	C3C-C2C	2.44	1.41	1.36
14	B3	1840	CLA	O2A-CGA	2.44	1.40	1.33
14	B6	806	CLA	C3D-C2D	2.44	1.44	1.39
14	B5	1833	CLA	CHB-C4A	2.44	1.36	1.33
16	A1	847	BCR	C30-C25	2.44	1.57	1.53
14	A1	815	CLA	O2A-CGA	2.44	1.40	1.33
14	B4	823	CLA	C3D-C2D	2.44	1.44	1.39
14	B3	1808	CLA	O2D-CGD	2.44	1.39	1.33
14	J6	1101	CLA	O2A-CGA	2.44	1.40	1.33
14	A1	818	CLA	O2A-CGA	2.44	1.40	1.33
14	B1	831	CLA	C3D-C2D	2.44	1.44	1.39
14	A4	837	CLA	C3D-C2D	2.44	1.44	1.39
14	A3	838	CLA	C3D-C2D	2.44	1.44	1.39
14	B1	819	CLA	C3D-C2D	2.44	1.44	1.39
14	B4	801	CLA	C3C-C2C	2.44	1.41	1.36
14	B5	1805	CLA	C1C-C2C	2.44	1.49	1.44
14	B3	1824	CLA	C3D-C2D	2.44	1.44	1.39
14	A4	841	CLA	C3D-C2D	2.44	1.44	1.39
14	B2	823	CLA	C3C-C2C	2.44	1.41	1.36
14	A5	830	CLA	O2D-CGD	2.44	1.39	1.33
14	B5	1841	CLA	CHB-C4A	2.44	1.36	1.33
14	A6	1619	CLA	O2A-CGA	2.44	1.40	1.33
14	A6	1621	CLA	OBD-CAD	2.45	1.25	1.22
17	A1	848	LHG	P-O6	2.45	1.69	1.59
14	L6	206	CLA	C3D-C2D	2.45	1.44	1.39
14	A6	1623	CLA	O2D-CGD	2.45	1.39	1.33
14	B6	825	CLA	O2D-CGD	2.45	1.39	1.33
14	A2	1604	CLA	O2D-CGD	2.45	1.39	1.33
14	B6	803	CLA	C3C-C2C	2.45	1.41	1.36
14	B2	821	CLA	C3D-C2D	2.45	1.44	1.39
14	B1	810	CLA	O2D-CGD	2.45	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	K5	102	CLA	C3D-C2D	2.45	1.44	1.39
14	B4	828	CLA	O2D-CGD	2.45	1.39	1.33
14	B6	810	CLA	O2A-CGA	2.45	1.40	1.33
14	A2	1621	CLA	CHB-C4A	2.45	1.36	1.33
14	A3	824	CLA	OBD-CAD	2.45	1.25	1.22
14	B6	838	CLA	C3C-C2C	2.45	1.41	1.36
14	B5	1823	CLA	C3C-C2C	2.45	1.41	1.36
14	J6	1102	CLA	C3D-C2D	2.45	1.44	1.39
14	A4	839	CLA	C3D-C2D	2.45	1.44	1.39
14	L3	203	CLA	C1C-C2C	2.45	1.49	1.44
14	J4	101	CLA	C3C-C2C	2.45	1.41	1.36
14	B4	808	CLA	OBD-CAD	2.45	1.25	1.22
14	I1	101	CLA	OBD-CAD	2.45	1.25	1.22
14	A3	806	CLA	C3D-C2D	2.45	1.44	1.39
14	B5	1839	CLA	C3C-C2C	2.45	1.42	1.36
14	B2	827	CLA	C2-C3	2.45	1.39	1.33
14	B1	823	CLA	C3D-C2D	2.45	1.44	1.39
14	A1	802	CLA	O2A-CGA	2.45	1.40	1.33
14	B5	1824	CLA	C3C-C2C	2.45	1.42	1.36
16	A4	845	BCR	C30-C25	2.45	1.57	1.53
14	A3	819	CLA	CHB-C4A	2.45	1.36	1.33
14	B3	1808	CLA	OBD-CAD	2.45	1.25	1.22
14	A1	814	CLA	C3C-C2C	2.45	1.42	1.36
14	A6	1638	CLA	O2D-CGD	2.45	1.39	1.33
14	B5	1822	CLA	C3C-C2C	2.45	1.42	1.36
14	A4	829	CLA	C3D-C2D	2.45	1.44	1.39
14	B4	801	CLA	C1C-C2C	2.45	1.49	1.44
14	B1	822	CLA	C3C-C2C	2.45	1.42	1.36
14	B5	1824	CLA	C3D-C2D	2.46	1.44	1.39
14	A1	821	CLA	C3C-C2C	2.46	1.42	1.36
14	B1	809	CLA	OBD-CAD	2.46	1.25	1.22
14	A1	817	CLA	O2A-CGA	2.46	1.40	1.33
14	B2	820	CLA	C3C-C2C	2.46	1.42	1.36
14	B6	824	CLA	C3C-C2C	2.46	1.42	1.36
14	B4	821	CLA	C3C-C2C	2.46	1.42	1.36
14	B4	852	CLA	O2A-CGA	2.46	1.40	1.33
17	A5	851	LHG	P-O6	2.46	1.69	1.59
14	B1	816	CLA	O2D-CGD	2.46	1.39	1.33
14	B4	829	CLA	C1C-C2C	2.46	1.49	1.44
14	A3	842	CLA	O2D-CGD	2.46	1.39	1.33
17	A5	852	LHG	P-O3	2.46	1.69	1.59
14	B4	830	CLA	C2-C3	2.46	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B4	810	CLA	O2D-CGD	2.46	1.39	1.33
14	A5	841	CLA	O2D-CGD	2.46	1.39	1.33
14	B5	1825	CLA	C3D-C2D	2.46	1.44	1.39
14	J5	101	CLA	C3C-C2C	2.46	1.42	1.36
14	A2	1608	CLA	O2A-CGA	2.46	1.40	1.33
14	B6	839	CLA	CHB-C4A	2.46	1.36	1.33
14	A4	823	CLA	C3C-C2C	2.46	1.42	1.36
14	B5	1827	CLA	C3C-C2C	2.46	1.42	1.36
14	B6	838	CLA	O2A-CGA	2.46	1.40	1.33
14	A1	829	CLA	O2D-CGD	2.46	1.39	1.33
14	A1	836	CLA	C3D-C2D	2.46	1.44	1.39
14	L2	202	CLA	CHB-C4A	2.46	1.36	1.33
14	B5	1828	CLA	O2D-CGD	2.46	1.39	1.33
14	A3	836	CLA	C3D-C2D	2.46	1.44	1.39
14	L5	204	CLA	C1C-C2C	2.47	1.49	1.44
14	B1	854	CLA	CHC-C1C	2.47	1.42	1.35
14	B4	803	CLA	C3D-C2D	2.47	1.44	1.39
14	B2	818	CLA	O2D-CGD	2.47	1.39	1.33
14	A5	822	CLA	C3D-C2D	2.47	1.44	1.39
14	A2	1615	CLA	O2A-CGA	2.47	1.40	1.33
14	B6	819	CLA	O2A-CGA	2.47	1.40	1.33
14	B6	815	CLA	O2D-CGD	2.47	1.39	1.33
14	A3	818	CLA	O2A-CGA	2.47	1.40	1.33
14	B5	1829	CLA	C1C-C2C	2.47	1.49	1.44
14	A2	1621	CLA	O2D-CGD	2.47	1.39	1.33
14	A2	1620	CLA	O2A-CGA	2.47	1.40	1.33
14	B1	826	CLA	C3C-C2C	2.47	1.42	1.36
14	B4	802	CLA	O2D-CGD	2.47	1.39	1.33
14	A5	815	CLA	C3D-C2D	2.47	1.44	1.39
14	B2	833	CLA	C3C-C2C	2.47	1.42	1.36
14	A2	1601	CLA	C3C-C2C	2.47	1.42	1.36
14	B5	1840	CLA	O2A-CGA	2.47	1.40	1.33
14	B5	1813	CLA	C3C-C2C	2.47	1.42	1.36
14	L1	201	CLA	C3D-C2D	2.47	1.44	1.39
14	B4	836	CLA	C3D-C2D	2.47	1.44	1.39
14	A5	807	CLA	O2A-CGA	2.47	1.40	1.33
14	B3	1837	CLA	C3C-C2C	2.47	1.42	1.36
14	B1	820	CLA	O2D-CGD	2.47	1.39	1.33
14	A3	832	CLA	C3D-C2D	2.47	1.44	1.39
14	A2	1615	CLA	C3D-C2D	2.47	1.44	1.39
14	B2	831	CLA	C3C-C2C	2.47	1.42	1.36
14	B1	832	CLA	CHB-C4A	2.47	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B5	1838	CLA	C3D-C2D	2.47	1.44	1.39
14	L6	206	CLA	C1C-C2C	2.47	1.49	1.44
14	B5	1837	CLA	C3D-C2D	2.47	1.44	1.39
14	L1	205	CLA	C1C-C2C	2.48	1.49	1.44
14	B4	840	CLA	C3C-C2C	2.48	1.42	1.36
14	A6	1607	CLA	O2D-CGD	2.48	1.39	1.33
14	A5	821	CLA	O2A-CGA	2.48	1.40	1.33
14	B6	837	CLA	C3C-C2C	2.48	1.42	1.36
14	A6	1615	CLA	C3D-C2D	2.48	1.44	1.39
14	B6	812	CLA	O2D-CGD	2.48	1.39	1.33
14	B5	1801	CLA	C3D-C2D	2.48	1.44	1.39
14	B1	824	CLA	C3D-C2D	2.48	1.44	1.39
14	B1	803	CLA	C3C-C2C	2.48	1.42	1.36
16	A1	844	BCR	C1-C6	2.48	1.57	1.53
14	L5	203	CLA	O2A-CGA	2.48	1.40	1.33
14	B3	1801	CLA	C3D-C2D	2.48	1.44	1.39
14	B6	834	CLA	C3C-C2C	2.48	1.42	1.36
14	B2	837	CLA	O2A-CGA	2.48	1.40	1.33
14	B5	1807	CLA	OBD-CAD	2.48	1.25	1.22
14	K1	1401	CLA	C3D-C2D	2.48	1.44	1.39
14	B6	827	CLA	O2D-CGD	2.48	1.39	1.33
14	A6	1630	CLA	C3D-C2D	2.48	1.44	1.39
14	B3	1818	CLA	O2D-CGD	2.48	1.39	1.33
14	A4	819	CLA	O2D-CGD	2.48	1.39	1.33
14	B4	808	CLA	O2D-CGD	2.48	1.39	1.33
14	A6	1619	CLA	CHB-C4A	2.48	1.36	1.33
14	B4	834	CLA	C3C-C2C	2.48	1.42	1.36
14	A3	815	CLA	C3D-C2D	2.48	1.44	1.39
14	B3	1804	CLA	C1C-C2C	2.48	1.49	1.44
14	L2	202	CLA	O2A-CGA	2.48	1.40	1.33
14	A1	835	CLA	C3D-C2D	2.48	1.44	1.39
14	B1	817	CLA	C3D-C2D	2.48	1.44	1.39
14	A3	821	CLA	O2A-CGA	2.49	1.40	1.33
14	B3	1837	CLA	O2D-CGD	2.49	1.39	1.33
14	B6	828	CLA	C2-C3	2.49	1.39	1.33
14	B6	834	CLA	C3D-C2D	2.49	1.44	1.39
14	B1	806	CLA	C3D-C2D	2.49	1.44	1.39
14	B5	1830	CLA	C2-C3	2.49	1.39	1.33
14	A2	1605	CLA	O2A-CGA	2.49	1.40	1.33
14	A1	811	CLA	C3D-C2D	2.49	1.44	1.39
14	B6	823	CLA	C3D-C2D	2.49	1.44	1.39
14	A2	1603	CLA	C1C-C2C	2.49	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A2	1609	CLA	O2A-CGA	2.49	1.40	1.33
14	A2	1603	CLA	C3C-C2C	2.49	1.42	1.36
14	A4	820	CLA	O2A-CGA	2.49	1.40	1.33
14	A5	826	CLA	OBD-CAD	2.49	1.25	1.22
14	B1	853	CLA	C3D-C2D	2.49	1.44	1.39
14	A1	822	CLA	O2D-CGD	2.49	1.39	1.33
14	B2	824	CLA	C3C-C2C	2.49	1.42	1.36
14	A3	843	CLA	OBD-CAD	2.49	1.25	1.22
14	A2	1625	CLA	O2D-CGD	2.49	1.39	1.33
14	B3	1840	CLA	C3D-C2D	2.49	1.44	1.39
14	B1	821	CLA	C3D-C2D	2.49	1.44	1.39
14	B5	1814	CLA	O2D-CGD	2.49	1.39	1.33
14	A5	803	CLA	O2A-CGA	2.49	1.40	1.33
14	B1	830	CLA	C3D-C2D	2.49	1.44	1.39
14	K2	1401	CLA	C3D-C2D	2.49	1.44	1.39
14	A3	826	CLA	OBD-CAD	2.49	1.25	1.22
16	A6	1643	BCR	C1-C6	2.49	1.57	1.53
14	B2	830	CLA	CHB-C4A	2.49	1.36	1.33
14	A6	1607	CLA	O2A-CGA	2.49	1.40	1.33
14	B1	825	CLA	C3C-C2C	2.49	1.42	1.36
14	A3	812	CLA	C3D-C2D	2.49	1.44	1.39
14	B1	823	CLA	C3C-C2C	2.49	1.42	1.36
14	K4	1401	CLA	C3D-C2D	2.49	1.44	1.39
14	L1	202	CLA	O2A-CGA	2.49	1.40	1.33
14	B2	825	CLA	O2D-CGD	2.49	1.39	1.33
14	B3	1830	CLA	C2-C3	2.50	1.39	1.33
17	A6	1650	LHG	P-O3	2.50	1.69	1.59
14	B1	804	CLA	O2D-CGD	2.50	1.39	1.33
14	B1	839	CLA	C3C-C2C	2.50	1.42	1.36
14	B2	826	CLA	C1C-C2C	2.50	1.49	1.44
14	A5	832	CLA	C3D-C2D	2.50	1.44	1.39
14	B6	808	CLA	O2D-CGD	2.50	1.39	1.33
14	B4	841	CLA	O2D-CGD	2.50	1.39	1.33
14	A2	1644	CLA	OBD-CAD	2.50	1.25	1.22
14	B2	809	CLA	CHC-C1C	2.50	1.42	1.35
14	L6	203	CLA	OBD-CAD	2.50	1.25	1.22
14	B5	1826	CLA	C3C-C2C	2.50	1.42	1.36
14	B4	823	CLA	C3C-C2C	2.50	1.42	1.36
14	B6	810	CLA	CHC-C1C	2.50	1.42	1.35
14	A6	1636	CLA	O2A-CGA	2.50	1.40	1.33
14	L6	208	CLA	C3D-C2D	2.50	1.44	1.39
14	A5	809	CLA	O2D-CGD	2.50	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B3	1807	CLA	OBD-CAD	2.50	1.25	1.22
14	B3	1812	CLA	CHC-C1C	2.50	1.42	1.35
14	A5	828	CLA	O2D-CGD	2.50	1.39	1.33
14	B4	821	CLA	O2D-CGD	2.50	1.39	1.33
14	B2	809	CLA	O2A-CGA	2.50	1.40	1.33
14	A5	805	CLA	OBD-CAD	2.50	1.25	1.22
14	A6	1613	CLA	C3D-C2D	2.50	1.44	1.39
14	A4	841	CLA	OBD-CAD	2.51	1.25	1.22
14	B5	1830	CLA	O2D-CGD	2.51	1.39	1.33
14	A4	814	CLA	C3D-C2D	2.51	1.44	1.39
14	A3	810	CLA	O2D-CGD	2.51	1.39	1.33
14	A2	1631	CLA	O2D-CGD	2.51	1.39	1.33
17	A1	849	LHG	P-O3	2.51	1.69	1.59
14	B2	806	CLA	OBD-CAD	2.51	1.25	1.22
14	A1	828	CLA	O2D-CGD	2.51	1.39	1.33
14	B2	811	CLA	O2D-CGD	2.51	1.39	1.33
14	B3	1825	CLA	C3D-C2D	2.51	1.44	1.39
14	B3	1836	CLA	C3C-C2C	2.51	1.42	1.36
14	B3	1803	CLA	O2D-CGD	2.51	1.39	1.33
14	B2	820	CLA	C3D-C2D	2.51	1.44	1.39
14	A5	807	CLA	O2D-CGD	2.51	1.39	1.33
14	B2	805	CLA	OBD-CAD	2.51	1.25	1.22
14	B6	832	CLA	C3C-C2C	2.51	1.42	1.36
14	B4	813	CLA	C3C-C2C	2.51	1.42	1.36
14	B1	802	CLA	O2D-CGD	2.51	1.39	1.33
14	A3	802	CLA	O2D-CGD	2.51	1.39	1.33
14	A6	1622	CLA	C3D-C2D	2.51	1.44	1.39
14	B4	803	CLA	O2D-CGD	2.51	1.39	1.33
14	B1	807	CLA	C3D-C2D	2.51	1.44	1.39
14	B4	822	CLA	C3C-C2C	2.51	1.42	1.36
14	B1	836	CLA	C3D-C2D	2.51	1.44	1.39
14	B4	812	CLA	O2A-CGA	2.51	1.40	1.33
14	B5	1833	CLA	OBD-CAD	2.51	1.25	1.22
14	B6	821	CLA	C3D-C2D	2.51	1.44	1.39
14	A2	1639	CLA	C3D-C2D	2.51	1.44	1.39
14	B1	813	CLA	O2D-CGD	2.51	1.39	1.33
14	A5	829	CLA	C3B-C2B	2.51	1.43	1.40
14	A3	806	CLA	O2A-CGA	2.51	1.40	1.33
14	A1	806	CLA	O2A-CGA	2.52	1.40	1.33
14	B4	812	CLA	CHC-C1C	2.52	1.42	1.35
14	A6	1628	CLA	OBD-CAD	2.52	1.25	1.22
14	A2	1609	CLA	O2D-CGD	2.52	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B4	826	CLA	C3C-C2C	2.52	1.42	1.36
14	K3	1401	CLA	O2D-CGD	2.52	1.39	1.33
14	K6	1401	CLA	O2D-CGD	2.52	1.39	1.33
14	B5	1842	CLA	O2A-CGA	2.52	1.40	1.33
14	A6	1633	CLA	O2A-CGA	2.52	1.40	1.33
14	B3	1839	CLA	C3C-C2C	2.52	1.42	1.36
14	B3	1828	CLA	O2D-CGD	2.52	1.39	1.33
14	B3	1827	CLA	C3C-C2C	2.52	1.42	1.36
14	B1	838	CLA	C3C-C2C	2.52	1.42	1.36
14	B4	816	CLA	O2D-CGD	2.52	1.39	1.33
14	A1	839	CLA	C3D-C2D	2.52	1.44	1.39
14	B3	1805	CLA	C3D-C2D	2.52	1.44	1.39
14	J3	101	CLA	C3D-C2D	2.52	1.44	1.39
14	A2	1634	CLA	C3D-C2D	2.52	1.44	1.39
14	B6	820	CLA	C3D-C2D	2.52	1.44	1.39
14	A2	1638	CLA	O2A-CGA	2.52	1.40	1.33
14	B6	826	CLA	O2D-CGD	2.52	1.39	1.33
16	A1	843	BCR	C30-C25	2.52	1.57	1.53
14	B1	825	CLA	OBD-CAD	2.53	1.25	1.22
14	A3	805	CLA	OBD-CAD	2.53	1.25	1.22
14	A4	835	CLA	O2A-CGA	2.53	1.40	1.33
14	B2	837	CLA	C3C-C2C	2.53	1.42	1.36
14	K1	1401	CLA	O2D-CGD	2.53	1.39	1.33
16	A5	845	BCR	C1-C6	2.53	1.57	1.53
14	B1	801	CLA	O2D-CGD	2.53	1.39	1.33
14	K4	1401	CLA	O2D-CGD	2.53	1.39	1.33
14	A3	834	CLA	CHB-C4A	2.53	1.36	1.33
14	L2	205	CLA	C1C-C2C	2.53	1.49	1.44
14	B4	821	CLA	C3D-C2D	2.53	1.44	1.39
17	A4	851	LHG	P-O3	2.53	1.69	1.59
14	B3	1819	CLA	O2D-CGD	2.53	1.39	1.33
14	B6	831	CLA	CHB-C4A	2.53	1.36	1.33
14	A2	1616	CLA	C3D-C2D	2.53	1.44	1.39
14	B6	818	CLA	O2D-CGD	2.53	1.39	1.33
14	L6	202	CLA	O2D-CGD	2.53	1.39	1.33
14	A1	838	CLA	O2A-CGA	2.53	1.40	1.33
14	B1	829	CLA	O2D-CGD	2.53	1.39	1.33
14	A6	1637	CLA	C3D-C2D	2.53	1.44	1.39
14	B2	833	CLA	C3D-C2D	2.53	1.44	1.39
14	B5	1836	CLA	C3C-C2C	2.53	1.42	1.36
16	A1	844	BCR	C30-C25	2.53	1.57	1.53
14	I6	101	CLA	C3D-C2D	2.53	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	832	CLA	O2D-CGD	2.53	1.39	1.33
14	B5	1812	CLA	CHC-C1C	2.53	1.42	1.35
14	B1	822	CLA	C3D-C2D	2.53	1.44	1.39
14	A3	802	CLA	C1C-C2C	2.53	1.49	1.44
16	A2	1649	BCR	C1-C6	2.53	1.57	1.53
14	A1	833	CLA	C3D-C2D	2.53	1.44	1.39
14	B5	1820	CLA	C3B-C2B	2.53	1.43	1.40
14	A3	829	CLA	C3D-C2D	2.54	1.44	1.39
14	B2	805	CLA	O2D-CGD	2.54	1.39	1.33
14	B3	1841	CLA	CHB-C4A	2.54	1.36	1.33
14	B3	1815	CLA	C3D-C2D	2.54	1.44	1.39
14	B2	822	CLA	C3D-C2D	2.54	1.44	1.39
14	A2	1603	CLA	O2D-CGD	2.54	1.39	1.33
14	K6	1401	CLA	C3D-C2D	2.54	1.44	1.39
14	B5	1811	CLA	O2D-CGD	2.54	1.39	1.33
14	X5	101	CLA	C3D-C2D	2.54	1.44	1.39
14	A6	1624	CLA	O2D-CGD	2.54	1.39	1.33
14	A5	830	CLA	OBD-CAD	2.54	1.25	1.22
14	A6	1625	CLA	O2A-CGA	2.54	1.40	1.33
14	A5	843	CLA	O2A-CGA	2.54	1.40	1.33
14	A4	805	CLA	O2A-CGA	2.54	1.40	1.33
14	F1	1301	CLA	C3D-C2D	2.54	1.44	1.39
14	B4	841	CLA	CHB-C4A	2.54	1.36	1.33
14	A1	838	CLA	O2D-CGD	2.54	1.39	1.33
17	A2	1654	LHG	P-O3	2.54	1.69	1.59
14	A3	829	CLA	OBD-CAD	2.54	1.25	1.22
14	B4	833	CLA	C3D-C2D	2.54	1.44	1.39
14	B4	827	CLA	C3C-C2C	2.54	1.42	1.36
14	B6	827	CLA	C1C-C2C	2.54	1.49	1.44
14	L1	207	CLA	C3D-C2D	2.54	1.44	1.39
14	B6	805	CLA	C3D-C2D	2.54	1.44	1.39
14	A1	828	CLA	C3B-C2B	2.54	1.43	1.40
14	B4	836	CLA	C3C-C2C	2.54	1.42	1.36
14	A5	818	CLA	O2A-CGA	2.54	1.40	1.33
14	A5	802	CLA	O2D-CGD	2.54	1.39	1.33
14	B2	827	CLA	O2D-CGD	2.54	1.39	1.33
14	B1	854	CLA	O2A-CGA	2.54	1.40	1.33
14	B2	807	CLA	O2D-CGD	2.54	1.39	1.33
14	A3	825	CLA	O2D-CGD	2.55	1.39	1.33
14	B3	1823	CLA	C3D-C2D	2.55	1.44	1.39
14	A3	823	CLA	O2D-CGD	2.55	1.39	1.33
14	B3	1822	CLA	C3D-C2D	2.55	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B1	835	CLA	C3D-C2D	2.55	1.44	1.39
14	B6	831	CLA	C3D-C2D	2.55	1.44	1.39
14	L5	206	CLA	C3D-C2D	2.55	1.44	1.39
14	B6	825	CLA	C3C-C2C	2.55	1.42	1.36
14	J2	101	CLA	C3C-C2C	2.55	1.42	1.36
14	B5	1841	CLA	OBD-CAD	2.55	1.25	1.22
16	A3	849	BCR	C30-C25	2.55	1.57	1.53
14	A4	820	CLA	OBD-CAD	2.55	1.26	1.22
14	B2	806	CLA	O2D-CGD	2.55	1.39	1.33
14	B4	811	CLA	O2D-CGD	2.55	1.39	1.33
14	B5	1833	CLA	C3D-C2D	2.55	1.44	1.39
14	A2	1614	CLA	C3D-C2D	2.55	1.44	1.39
14	A6	1629	CLA	O2D-CGD	2.55	1.39	1.33
14	A4	805	CLA	C3D-C2D	2.55	1.44	1.39
14	A6	1622	CLA	O2A-CGA	2.55	1.40	1.33
14	B3	1812	CLA	O2A-CGA	2.55	1.40	1.33
14	A6	1640	CLA	O2D-CGD	2.55	1.39	1.33
14	B6	826	CLA	C3D-C2D	2.55	1.44	1.39
14	B5	1821	CLA	O2D-CGD	2.55	1.39	1.33
14	A3	819	CLA	O2D-CGD	2.55	1.39	1.33
14	B3	1809	CLA	CHC-C1C	2.55	1.42	1.35
14	B1	835	CLA	C3C-C2C	2.55	1.42	1.36
14	B4	818	CLA	C3D-C2D	2.55	1.44	1.39
14	B2	816	CLA	O2D-CGD	2.55	1.39	1.33
14	B3	1826	CLA	OBD-CAD	2.55	1.26	1.22
14	A3	834	CLA	O2A-CGA	2.55	1.40	1.33
14	A2	1640	CLA	O2D-CGD	2.55	1.39	1.33
14	M1	1201	CLA	OBD-CAD	2.55	1.26	1.22
14	B1	825	CLA	C3D-C2D	2.55	1.44	1.39
14	B6	809	CLA	O2D-CGD	2.55	1.39	1.33
14	B4	840	CLA	O2A-CGA	2.55	1.40	1.33
14	A3	807	CLA	O2A-CGA	2.55	1.40	1.33
14	B6	802	CLA	C1C-C2C	2.55	1.49	1.44
14	B4	830	CLA	O2D-CGD	2.55	1.39	1.33
14	B4	801	CLA	O2D-CGD	2.55	1.39	1.33
14	J2	101	CLA	C3D-C2D	2.56	1.44	1.39
14	A3	837	CLA	O2A-CGA	2.56	1.40	1.33
14	B1	840	CLA	O2D-CGD	2.56	1.39	1.33
14	A5	836	CLA	O2A-CGA	2.56	1.40	1.33
16	A3	847	BCR	C1-C6	2.56	1.57	1.53
14	F6	202	CLA	C3D-C2D	2.56	1.44	1.39
14	B1	819	CLA	C3B-C2B	2.56	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B3	1820	CLA	O2D-CGD	2.56	1.39	1.33
14	B4	839	CLA	C3C-C2C	2.56	1.42	1.36
14	B5	1812	CLA	O2A-CGA	2.56	1.40	1.33
14	B2	839	CLA	O2A-CGA	2.56	1.40	1.33
14	B5	1826	CLA	C3D-C2D	2.56	1.44	1.39
14	A5	842	CLA	OBD-CAD	2.56	1.26	1.22
14	B6	820	CLA	O2A-CGA	2.56	1.40	1.33
14	B5	1818	CLA	C3D-C2D	2.56	1.44	1.39
14	B3	1814	CLA	C3D-C2D	2.56	1.44	1.39
14	B2	811	CLA	C3D-C2D	2.56	1.44	1.39
14	A2	1623	CLA	OBD-CAD	2.56	1.26	1.22
14	B3	1826	CLA	C3D-C2D	2.56	1.44	1.39
14	I1	101	CLA	O2A-CGA	2.56	1.40	1.33
16	A6	1645	BCR	C30-C25	2.56	1.57	1.53
14	A3	822	CLA	O2A-CGA	2.56	1.40	1.33
14	B3	1841	CLA	OBD-CAD	2.56	1.26	1.22
14	A6	1613	CLA	O2D-CGD	2.56	1.39	1.33
14	B5	1822	CLA	C3D-C2D	2.56	1.44	1.39
14	K2	1401	CLA	O2D-CGD	2.56	1.39	1.33
14	A4	821	CLA	C3D-C2D	2.56	1.44	1.39
14	A5	829	CLA	C3D-C2D	2.57	1.44	1.39
14	A5	812	CLA	C3D-C2D	2.57	1.44	1.39
14	A1	834	CLA	O2A-CGA	2.57	1.40	1.33
14	B2	808	CLA	O2D-CGD	2.57	1.39	1.33
14	A5	826	CLA	O2D-CGD	2.57	1.39	1.33
14	B3	1822	CLA	O2A-CGA	2.57	1.40	1.33
14	B1	828	CLA	C1C-C2C	2.57	1.49	1.44
14	A4	818	CLA	CHB-C4A	2.57	1.36	1.33
14	I6	101	CLA	CHC-C1C	2.57	1.42	1.35
14	B5	1809	CLA	O2D-CGD	2.57	1.39	1.33
14	I6	101	CLA	O2D-CGD	2.57	1.39	1.33
14	A3	831	CLA	O2D-CGD	2.57	1.39	1.33
14	A3	832	CLA	O2D-CGD	2.57	1.39	1.33
14	A4	828	CLA	O2D-CGD	2.57	1.39	1.33
14	A1	825	CLA	OBD-CAD	2.57	1.26	1.22
14	B1	829	CLA	C2-C3	2.57	1.39	1.33
14	A4	822	CLA	O2D-CGD	2.57	1.39	1.33
16	A2	1647	BCR	C1-C6	2.57	1.57	1.53
14	A4	802	CLA	O2A-CGA	2.57	1.40	1.33
14	A1	820	CLA	OBD-CAD	2.57	1.26	1.22
14	B3	1829	CLA	CHB-C4A	2.57	1.36	1.33
14	A5	828	CLA	CHB-C4A	2.57	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B5	1805	CLA	C3C-C2C	2.57	1.42	1.36
14	A6	1612	CLA	C3D-C2D	2.57	1.44	1.39
14	A6	1626	CLA	O2D-CGD	2.57	1.39	1.33
14	A4	817	CLA	O2A-CGA	2.57	1.40	1.33
14	B1	832	CLA	C3D-C2D	2.57	1.44	1.39
14	B4	834	CLA	CHB-C4A	2.57	1.36	1.33
14	B2	803	CLA	C3C-C2C	2.57	1.42	1.36
16	B2	842	BCR	C26-C25	2.57	1.38	1.34
14	A2	1636	CLA	O2D-CGD	2.57	1.39	1.33
14	B3	1829	CLA	C1C-C2C	2.58	1.49	1.44
14	A2	1643	CLA	O2D-CGD	2.58	1.39	1.33
16	A4	846	BCR	C30-C25	2.58	1.57	1.53
14	A1	827	CLA	O2D-CGD	2.58	1.39	1.33
14	B1	814	CLA	C3D-C2D	2.58	1.44	1.39
14	B3	1833	CLA	C3D-C2D	2.58	1.44	1.39
14	B5	1836	CLA	C3D-C2D	2.58	1.44	1.39
14	B4	807	CLA	C3D-C2D	2.58	1.44	1.39
14	B6	831	CLA	OBD-CAD	2.58	1.26	1.22
14	B5	1839	CLA	C3D-C2D	2.58	1.44	1.39
14	L2	207	CLA	C3D-C2D	2.58	1.44	1.39
14	B4	814	CLA	C3D-C2D	2.58	1.44	1.39
14	B6	818	CLA	C3B-C2B	2.58	1.43	1.40
14	A5	808	CLA	O2D-CGD	2.58	1.39	1.33
14	B6	805	CLA	C3C-C2C	2.58	1.42	1.36
14	A2	1630	CLA	OBD-CAD	2.58	1.26	1.22
14	A4	804	CLA	OBD-CAD	2.58	1.26	1.22
14	A3	817	CLA	O2D-CGD	2.58	1.39	1.33
16	A4	846	BCR	C1-C6	2.58	1.57	1.53
14	K5	101	CLA	OBD-CAD	2.58	1.26	1.22
14	B6	802	CLA	O2D-CGD	2.58	1.39	1.33
14	B1	817	CLA	O2D-CGD	2.58	1.39	1.33
14	B1	840	CLA	CHB-C4A	2.58	1.36	1.33
14	B4	837	CLA	CHB-C4A	2.58	1.36	1.33
14	A5	829	CLA	O2D-CGD	2.59	1.39	1.33
14	B5	1815	CLA	C3D-C2D	2.59	1.44	1.39
14	B4	814	CLA	O2D-CGD	2.59	1.39	1.33
14	A1	807	CLA	O2D-CGD	2.59	1.39	1.33
14	A6	1625	CLA	O2D-CGD	2.59	1.39	1.33
14	B2	838	CLA	OBD-CAD	2.59	1.26	1.22
14	B2	830	CLA	C3D-C2D	2.59	1.44	1.39
14	A4	801	CLA	O2A-CGA	2.59	1.40	1.33
14	A3	825	CLA	O2A-CGA	2.59	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A1	825	CLA	O2D-CGD	2.59	1.39	1.33
14	A5	825	CLA	O2A-CGA	2.59	1.40	1.33
14	B1	811	CLA	O2D-CGD	2.59	1.39	1.33
14	B6	816	CLA	O2D-CGD	2.59	1.39	1.33
14	B4	819	CLA	CHB-C4A	2.59	1.36	1.33
14	B4	833	CLA	CHB-C4A	2.59	1.36	1.33
14	A6	1639	CLA	O2D-CGD	2.59	1.39	1.33
14	A1	836	CLA	O2D-CGD	2.59	1.39	1.33
14	B1	833	CLA	C3C-C2C	2.59	1.42	1.36
16	A1	842	BCR	C1-C6	2.59	1.57	1.53
14	B3	1807	CLA	C3D-C2D	2.59	1.44	1.39
14	A4	838	CLA	O2D-CGD	2.59	1.39	1.33
16	B1	843	BCR	C26-C25	2.59	1.38	1.34
14	A4	834	CLA	C3D-C2D	2.59	1.44	1.39
14	B2	812	CLA	C3D-C2D	2.59	1.44	1.39
14	B1	812	CLA	C3C-C2C	2.59	1.42	1.36
14	X4	102	CLA	C3D-C2D	2.59	1.44	1.39
14	J1	101	CLA	C3C-C2C	2.59	1.42	1.36
14	A1	839	CLA	OBD-CAD	2.59	1.26	1.22
14	B3	1814	CLA	O2D-CGD	2.59	1.39	1.33
14	B6	804	CLA	C3D-C2D	2.59	1.44	1.39
14	B5	1822	CLA	O2A-CGA	2.59	1.40	1.33
14	B6	811	CLA	C3C-C2C	2.59	1.42	1.36
14	B3	1812	CLA	OBD-CAD	2.59	1.26	1.22
14	B2	834	CLA	O2D-CGD	2.59	1.39	1.33
14	A3	826	CLA	O2D-CGD	2.59	1.39	1.33
14	A4	818	CLA	O2D-CGD	2.59	1.39	1.33
14	A5	821	CLA	OBD-CAD	2.60	1.26	1.22
14	B4	818	CLA	O2D-CGD	2.60	1.39	1.33
14	A5	819	CLA	O2D-CGD	2.60	1.39	1.33
14	A6	1631	CLA	O2D-CGD	2.60	1.39	1.33
14	A5	819	CLA	C3D-C2D	2.60	1.44	1.39
14	B1	809	CLA	CHC-C1C	2.60	1.42	1.35
14	B6	827	CLA	CHB-C4A	2.60	1.36	1.33
14	B4	833	CLA	OBD-CAD	2.60	1.26	1.22
14	A4	825	CLA	OBD-CAD	2.60	1.26	1.22
14	A2	1624	CLA	C3D-C2D	2.60	1.44	1.39
14	A4	837	CLA	O2D-CGD	2.60	1.39	1.33
14	A6	1611	CLA	O2D-CGD	2.60	1.39	1.33
14	A6	1619	CLA	O2D-CGD	2.60	1.39	1.33
14	A6	1614	CLA	C3D-C2D	2.60	1.44	1.39
14	B1	821	CLA	O2A-CGA	2.60	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	802	CLA	C1C-C2C	2.60	1.49	1.44
14	B5	1814	CLA	C3D-C2D	2.60	1.44	1.39
14	B2	813	CLA	O2D-CGD	2.60	1.39	1.33
14	K5	102	CLA	O2D-CGD	2.60	1.39	1.33
16	A3	847	BCR	C30-C25	2.60	1.57	1.53
14	A4	836	CLA	C3D-C2D	2.60	1.44	1.39
14	A1	840	CLA	OBD-CAD	2.60	1.26	1.22
14	B2	819	CLA	O2A-CGA	2.60	1.40	1.33
14	B4	815	CLA	C3D-C2D	2.60	1.44	1.39
14	B4	809	CLA	O2D-CGD	2.60	1.39	1.33
14	A5	841	CLA	O2A-CGA	2.60	1.40	1.33
14	A4	821	CLA	O2A-CGA	2.60	1.40	1.33
14	B2	815	CLA	C3D-C2D	2.60	1.44	1.39
14	A2	1613	CLA	O2D-CGD	2.60	1.39	1.33
14	B3	1816	CLA	O2D-CGD	2.60	1.39	1.33
14	A3	828	CLA	OBD-CAD	2.61	1.26	1.22
14	A4	831	CLA	C3D-C2D	2.61	1.44	1.39
14	A4	840	CLA	O2A-CGA	2.61	1.40	1.33
14	A3	813	CLA	O2D-CGD	2.61	1.39	1.33
14	B4	833	CLA	O2D-CGD	2.61	1.39	1.33
14	A5	838	CLA	O2D-CGD	2.61	1.39	1.33
14	B4	852	CLA	C3D-C2D	2.61	1.44	1.39
14	F6	202	CLA	O2D-CGD	2.61	1.39	1.33
14	A1	821	CLA	O2A-CGA	2.61	1.40	1.33
14	B2	830	CLA	O2D-CGD	2.61	1.39	1.33
14	J4	102	CLA	OBD-CAD	2.61	1.26	1.22
14	A6	1617	CLA	O2D-CGD	2.61	1.39	1.33
14	B3	1811	CLA	O2D-CGD	2.61	1.39	1.33
14	A4	840	CLA	O2D-CGD	2.61	1.39	1.33
14	B6	817	CLA	O2D-CGD	2.61	1.39	1.33
14	B1	809	CLA	O2D-CGD	2.61	1.39	1.33
14	B5	1819	CLA	O2D-CGD	2.61	1.39	1.33
14	A5	813	CLA	O2D-CGD	2.62	1.39	1.33
14	A1	818	CLA	O2D-CGD	2.62	1.39	1.33
14	A3	811	CLA	O2D-CGD	2.62	1.39	1.33
14	B4	842	CLA	O2A-CGA	2.62	1.40	1.33
14	B4	805	CLA	C3C-C2C	2.62	1.42	1.36
14	A1	803	CLA	O2D-CGD	2.62	1.39	1.33
16	A3	849	BCR	C1-C6	2.62	1.57	1.53
14	B2	806	CLA	CHC-C1C	2.62	1.42	1.35
14	A2	1634	CLA	O2D-CGD	2.62	1.39	1.33
14	A4	823	CLA	OBD-CAD	2.62	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B4	826	CLA	C3D-C2D	2.62	1.44	1.39
14	B1	807	CLA	O2D-CGD	2.62	1.39	1.33
14	A1	810	CLA	O2D-CGD	2.62	1.39	1.33
14	A4	806	CLA	O2D-CGD	2.62	1.39	1.33
14	B6	809	CLA	OBD-CAD	2.62	1.26	1.22
14	A4	811	CLA	C3D-C2D	2.63	1.45	1.39
14	B5	1823	CLA	C3D-C2D	2.63	1.45	1.39
14	L1	206	CLA	CHB-C4A	2.63	1.36	1.33
14	A3	840	CLA	O2D-CGD	2.63	1.39	1.33
14	L5	205	CLA	CHB-C4A	2.63	1.36	1.33
16	B5	1845	BCR	C26-C25	2.63	1.39	1.34
14	B3	1835	CLA	O2D-CGD	2.63	1.39	1.33
14	B2	809	CLA	OBD-CAD	2.63	1.26	1.22
14	B5	1812	CLA	OBD-CAD	2.63	1.26	1.22
14	B6	812	CLA	C3D-C2D	2.63	1.45	1.39
14	B4	809	CLA	CHC-C1C	2.63	1.42	1.35
14	A1	806	CLA	O2D-CGD	2.63	1.39	1.33
14	A4	806	CLA	O2A-CGA	2.63	1.40	1.33
14	A2	1620	CLA	O2D-CGD	2.63	1.39	1.33
14	X6	1701	CLA	C3D-C2D	2.63	1.45	1.39
14	B6	824	CLA	C3D-C2D	2.63	1.45	1.39
14	A3	820	CLA	O2A-CGA	2.63	1.40	1.33
14	A5	810	CLA	O2D-CGD	2.63	1.39	1.33
14	A4	842	CLA	C3D-C2D	2.63	1.45	1.39
16	B2	850	BCR	C30-C25	2.63	1.57	1.53
14	L1	201	CLA	O2D-CGD	2.63	1.39	1.33
14	B2	836	CLA	C3C-C2C	2.63	1.42	1.36
14	A5	834	CLA	O2D-CGD	2.64	1.39	1.33
14	B1	854	CLA	OBD-CAD	2.64	1.26	1.22
14	B5	1811	CLA	OBD-CAD	2.64	1.26	1.22
14	A5	840	CLA	O2D-CGD	2.64	1.39	1.33
14	B2	815	CLA	O2D-CGD	2.64	1.39	1.33
14	B1	804	CLA	C3D-C2D	2.64	1.45	1.39
14	B3	1805	CLA	C3C-C2C	2.64	1.42	1.36
14	A3	842	CLA	O2A-CGA	2.64	1.41	1.33
14	B4	807	CLA	OBD-CAD	2.64	1.26	1.22
14	A4	839	CLA	O2D-CGD	2.64	1.39	1.33
14	B3	1838	CLA	C3D-C2D	2.64	1.45	1.39
14	F3	202	CLA	C3D-C2D	2.64	1.45	1.39
14	B5	1809	CLA	C3D-C2D	2.64	1.45	1.39
14	A3	830	CLA	OBD-CAD	2.64	1.26	1.22
14	A3	839	CLA	O2D-CGD	2.64	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A2	1645	CLA	OBD-CAD	2.64	1.26	1.22
16	A5	847	BCR	C30-C25	2.64	1.57	1.53
14	B4	841	CLA	OBD-CAD	2.64	1.26	1.22
14	A2	1626	CLA	OBD-CAD	2.64	1.26	1.22
16	B4	845	BCR	C26-C25	2.64	1.39	1.34
14	A3	818	CLA	O2D-CGD	2.64	1.39	1.33
14	L4	205	CLA	C3D-C2D	2.64	1.45	1.39
14	B4	822	CLA	O2A-CGA	2.64	1.41	1.33
14	B5	1837	CLA	O2D-CGD	2.64	1.39	1.33
14	B4	811	CLA	OBD-CAD	2.64	1.26	1.22
16	B6	843	BCR	C26-C25	2.64	1.39	1.34
14	B3	1811	CLA	OBD-CAD	2.64	1.26	1.22
14	B5	1819	CLA	CHB-C4A	2.64	1.36	1.33
14	B1	832	CLA	OBD-CAD	2.64	1.26	1.22
14	A6	1602	CLA	O2A-CGA	2.64	1.41	1.33
14	A4	834	CLA	O2D-CGD	2.64	1.39	1.33
14	A6	1629	CLA	C3D-C2D	2.64	1.45	1.39
14	B2	838	CLA	CHB-C4A	2.65	1.36	1.33
14	B3	1833	CLA	OBD-CAD	2.65	1.26	1.22
14	B3	1803	CLA	C3D-C2D	2.65	1.45	1.39
14	A2	1619	CLA	O2D-CGD	2.65	1.39	1.33
14	A5	814	CLA	C3D-C2D	2.65	1.45	1.39
14	B2	830	CLA	OBD-CAD	2.65	1.26	1.22
14	A5	804	CLA	O2D-CGD	2.65	1.39	1.33
14	B1	814	CLA	O2D-CGD	2.65	1.39	1.33
14	B6	810	CLA	OBD-CAD	2.65	1.26	1.22
14	A3	844	CLA	C3D-C2D	2.65	1.45	1.39
14	B3	1836	CLA	C3D-C2D	2.65	1.45	1.39
14	A5	822	CLA	O2A-CGA	2.65	1.41	1.33
14	A2	1624	CLA	O2A-CGA	2.65	1.41	1.33
14	A5	818	CLA	O2D-CGD	2.65	1.39	1.33
14	A4	831	CLA	O2A-CGA	2.65	1.41	1.33
14	A4	825	CLA	O2D-CGD	2.65	1.39	1.33
14	A6	1605	CLA	OBD-CAD	2.65	1.26	1.22
16	A2	1647	BCR	C30-C25	2.65	1.57	1.53
14	A2	1602	CLA	O2A-CGA	2.65	1.41	1.33
14	A2	1631	CLA	C3B-C2B	2.65	1.44	1.40
14	B3	1820	CLA	C3B-C2B	2.65	1.44	1.40
14	A5	817	CLA	O2D-CGD	2.65	1.39	1.33
14	B6	832	CLA	CHB-C4A	2.65	1.36	1.33
14	A4	819	CLA	O2A-CGA	2.65	1.41	1.33
14	B5	1835	CLA	OBD-CAD	2.65	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	811	CLA	O2D-CGD	2.65	1.39	1.33
14	B4	838	CLA	O2D-CGD	2.66	1.39	1.33
14	A4	824	CLA	O2A-CGA	2.66	1.41	1.33
14	B5	1831	CLA	C3B-C2B	2.66	1.44	1.40
14	B6	803	CLA	O2D-CGD	2.66	1.39	1.33
14	A3	812	CLA	O2A-CGA	2.66	1.41	1.33
14	A6	1610	CLA	O2D-CGD	2.66	1.39	1.33
14	A2	1631	CLA	OBD-CAD	2.66	1.26	1.22
14	B6	839	CLA	OBD-CAD	2.66	1.26	1.22
16	A4	844	BCR	C1-C6	2.66	1.57	1.53
14	A5	824	CLA	OBD-CAD	2.66	1.26	1.22
14	A2	1606	CLA	O2D-CGD	2.66	1.39	1.33
14	A4	810	CLA	O2D-CGD	2.66	1.39	1.33
14	X3	102	CLA	C3D-C2D	2.66	1.45	1.39
14	B5	1833	CLA	O2D-CGD	2.66	1.39	1.33
14	A3	829	CLA	O2D-CGD	2.66	1.39	1.33
14	A6	1604	CLA	O2D-CGD	2.66	1.39	1.33
14	A3	820	CLA	OBD-CAD	2.66	1.26	1.22
14	F2	204	CLA	OBD-CAD	2.66	1.26	1.22
14	A1	816	CLA	O2D-CGD	2.66	1.39	1.33
14	A6	1640	CLA	O2A-CGA	2.66	1.41	1.33
14	A1	827	CLA	OBD-CAD	2.66	1.26	1.22
14	A4	827	CLA	OBD-CAD	2.66	1.26	1.22
14	A3	829	CLA	C3B-C2B	2.66	1.44	1.40
14	A4	816	CLA	O2D-CGD	2.66	1.39	1.33
14	B1	836	CLA	OBD-CAD	2.66	1.26	1.22
14	B6	813	CLA	C3D-C2D	2.66	1.45	1.39
14	A5	801	CLA	O2A-CGA	2.66	1.41	1.33
14	A2	1627	CLA	O2D-CGD	2.66	1.39	1.33
14	B4	820	CLA	O2D-CGD	2.66	1.39	1.33
14	B6	828	CLA	O2D-CGD	2.67	1.39	1.33
14	A1	824	CLA	O2A-CGA	2.67	1.41	1.33
14	F3	202	CLA	O2D-CGD	2.67	1.39	1.33
14	B2	823	CLA	OBD-CAD	2.67	1.26	1.22
14	B6	835	CLA	O2D-CGD	2.67	1.39	1.33
14	A2	1620	CLA	OBD-CAD	2.67	1.26	1.22
14	A3	831	CLA	CHB-C4A	2.67	1.36	1.33
14	B2	831	CLA	CHB-C4A	2.67	1.36	1.33
14	B1	813	CLA	C3D-C2D	2.67	1.45	1.39
14	A3	827	CLA	O2A-CGA	2.67	1.41	1.33
14	B1	853	CLA	O2A-CGA	2.67	1.41	1.33
14	A6	1619	CLA	C3D-C2D	2.67	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A2	1633	CLA	O2D-CGD	2.67	1.39	1.33
14	B6	831	CLA	O2D-CGD	2.67	1.39	1.33
14	B4	812	CLA	OBD-CAD	2.67	1.26	1.22
14	A3	841	CLA	O2D-CGD	2.67	1.39	1.33
14	B5	1837	CLA	CHB-C4A	2.67	1.36	1.33
16	A6	1643	BCR	C30-C25	2.67	1.57	1.53
14	B6	817	CLA	CHB-C4A	2.67	1.36	1.33
14	B1	803	CLA	O2D-CGD	2.67	1.39	1.33
14	X2	1701	CLA	C3D-C2D	2.67	1.45	1.39
14	A6	1618	CLA	OBD-CAD	2.67	1.26	1.22
14	B2	801	CLA	C3D-C2D	2.67	1.45	1.39
14	B5	1834	CLA	CHB-C4A	2.67	1.36	1.33
14	B3	1809	CLA	O2D-CGD	2.67	1.39	1.33
14	A4	830	CLA	O2D-CGD	2.67	1.39	1.33
14	A4	813	CLA	C3D-C2D	2.67	1.45	1.39
14	B2	817	CLA	C3B-C2B	2.67	1.44	1.40
14	A4	811	CLA	O2A-CGA	2.67	1.41	1.33
14	A4	842	CLA	OBD-CAD	2.67	1.26	1.22
14	A2	1627	CLA	O2A-CGA	2.67	1.41	1.33
14	F1	1301	CLA	O2D-CGD	2.67	1.39	1.33
14	A6	1641	CLA	OBD-CAD	2.67	1.26	1.22
14	A2	1619	CLA	OBD-CAD	2.67	1.26	1.22
14	A5	821	CLA	CHB-C4A	2.67	1.36	1.33
14	B4	837	CLA	O2D-CGD	2.67	1.39	1.33
14	A5	835	CLA	O2D-CGD	2.68	1.39	1.33
14	F4	202	CLA	O2D-CGD	2.68	1.39	1.33
14	A6	1629	CLA	C3B-C2B	2.68	1.44	1.40
14	A1	823	CLA	OBD-CAD	2.68	1.26	1.22
14	B1	811	CLA	OBD-CAD	2.68	1.26	1.22
14	B1	806	CLA	C3C-C2C	2.68	1.42	1.36
14	B1	815	CLA	O2D-CGD	2.68	1.39	1.33
16	L5	201	BCR	C30-C25	2.68	1.57	1.53
14	B2	823	CLA	C3D-C2D	2.68	1.45	1.39
14	B1	801	CLA	C1C-C2C	2.68	1.49	1.44
14	A2	1607	CLA	OBD-CAD	2.68	1.26	1.22
14	B5	1820	CLA	O2D-CGD	2.68	1.39	1.33
14	B3	1833	CLA	O2D-CGD	2.68	1.39	1.33
14	B4	835	CLA	O2D-CGD	2.68	1.39	1.33
14	A2	1643	CLA	O2A-CGA	2.68	1.41	1.33
14	A2	1633	CLA	OBD-CAD	2.68	1.26	1.22
14	A1	817	CLA	O2D-CGD	2.68	1.39	1.33
14	B4	831	CLA	C3B-C2B	2.69	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A2	1625	CLA	O2A-CGA	2.69	1.41	1.33
14	F5	1301	CLA	C3D-C2D	2.69	1.45	1.39
14	A4	828	CLA	C3B-C2B	2.69	1.44	1.40
14	A1	801	CLA	O2A-CGA	2.69	1.41	1.33
14	A4	833	CLA	O2D-CGD	2.69	1.39	1.33
14	A3	808	CLA	O2D-CGD	2.69	1.39	1.33
14	B5	1818	CLA	O2D-CGD	2.69	1.39	1.33
14	J5	102	CLA	OBD-CAD	2.69	1.26	1.22
14	B5	1811	CLA	CHC-C1C	2.69	1.42	1.35
14	A1	828	CLA	OBD-CAD	2.69	1.26	1.22
14	A4	817	CLA	O2D-CGD	2.69	1.39	1.33
16	A5	845	BCR	C30-C25	2.69	1.57	1.53
14	A2	1628	CLA	O2D-CGD	2.69	1.39	1.33
14	B5	1815	CLA	O2D-CGD	2.69	1.39	1.33
14	B5	1838	CLA	O2D-CGD	2.69	1.39	1.33
14	A6	1628	CLA	O2D-CGD	2.69	1.39	1.33
14	A2	1623	CLA	CHB-C4A	2.69	1.36	1.33
14	B3	1831	CLA	C3B-C2B	2.69	1.44	1.40
14	A1	817	CLA	OBD-CAD	2.69	1.26	1.22
14	B6	811	CLA	CHB-C4A	2.70	1.36	1.33
14	A2	1612	CLA	O2D-CGD	2.70	1.39	1.33
14	A6	1608	CLA	O2D-CGD	2.70	1.40	1.33
14	A3	815	CLA	O2D-CGD	2.70	1.40	1.33
14	A3	801	CLA	O2A-CGA	2.70	1.41	1.33
14	A6	1641	CLA	C3D-C2D	2.70	1.45	1.39
14	B1	840	CLA	OBD-CAD	2.70	1.26	1.22
14	A4	803	CLA	O2D-CGD	2.70	1.40	1.33
14	A6	1632	CLA	CHC-C1C	2.70	1.43	1.35
14	A6	1631	CLA	OBD-CAD	2.70	1.26	1.22
14	F2	202	CLA	O2D-CGD	2.70	1.40	1.33
14	B4	819	CLA	O2D-CGD	2.70	1.40	1.33
14	A3	819	CLA	C3D-C2D	2.70	1.45	1.39
14	A5	831	CLA	OBD-CAD	2.70	1.26	1.22
14	A1	837	CLA	O2D-CGD	2.70	1.40	1.33
14	L6	207	CLA	CHB-C4A	2.70	1.36	1.33
14	B1	809	CLA	C3D-C2D	2.70	1.45	1.39
14	A2	1621	CLA	C3D-C2D	2.70	1.45	1.39
14	A1	804	CLA	OBD-CAD	2.70	1.26	1.22
14	A5	839	CLA	O2D-CGD	2.71	1.40	1.33
14	F5	1301	CLA	O2D-CGD	2.71	1.40	1.33
14	B3	1803	CLA	OBD-CAD	2.71	1.26	1.22
14	A4	832	CLA	CHC-C1C	2.71	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A1	828	CLA	C3D-C2D	2.71	1.45	1.39
14	A1	815	CLA	O2D-CGD	2.71	1.40	1.33
14	A3	823	CLA	OBD-CAD	2.71	1.26	1.22
14	A3	804	CLA	O2D-CGD	2.71	1.40	1.33
14	A6	1630	CLA	OBD-CAD	2.71	1.26	1.22
14	A6	1635	CLA	O2D-CGD	2.71	1.40	1.33
14	B1	818	CLA	O2D-CGD	2.71	1.40	1.33
14	A2	1634	CLA	O2A-CGA	2.71	1.41	1.33
14	B2	829	CLA	OBD-CAD	2.71	1.26	1.22
14	A5	833	CLA	CHC-C1C	2.71	1.43	1.35
14	A1	833	CLA	O2D-CGD	2.71	1.40	1.33
14	A4	809	CLA	O2D-CGD	2.71	1.40	1.33
14	B4	839	CLA	C3D-C2D	2.71	1.45	1.39
14	B6	809	CLA	CHC-C1C	2.71	1.43	1.35
14	J6	1102	CLA	O2D-CGD	2.71	1.40	1.33
14	F4	202	CLA	C3D-C2D	2.71	1.45	1.39
14	A3	828	CLA	O2D-CGD	2.71	1.40	1.33
14	B2	835	CLA	O2D-CGD	2.71	1.40	1.33
14	B5	1809	CLA	CHC-C1C	2.71	1.43	1.35
14	A3	831	CLA	OBD-CAD	2.71	1.26	1.22
14	A1	832	CLA	O2D-CGD	2.71	1.40	1.33
14	B5	1816	CLA	O2D-CGD	2.71	1.40	1.33
14	A6	1634	CLA	O2D-CGD	2.71	1.40	1.33
14	L6	202	CLA	C3D-C2D	2.71	1.45	1.39
14	B6	824	CLA	OBD-CAD	2.71	1.26	1.22
14	A2	1631	CLA	C3D-C2D	2.71	1.45	1.39
14	B1	819	CLA	O2D-CGD	2.71	1.40	1.33
14	A1	809	CLA	O2D-CGD	2.71	1.40	1.33
14	X1	1701	CLA	C3D-C2D	2.71	1.45	1.39
14	B6	811	CLA	O2D-CGD	2.71	1.40	1.33
14	A2	1635	CLA	CHC-C1C	2.72	1.43	1.35
14	A4	824	CLA	O2D-CGD	2.72	1.40	1.33
14	A6	1612	CLA	O2A-CGA	2.72	1.41	1.33
14	A4	830	CLA	OBD-CAD	2.72	1.26	1.22
14	A6	1618	CLA	O2D-CGD	2.72	1.40	1.33
14	A5	823	CLA	O2A-CGA	2.72	1.41	1.33
14	A5	812	CLA	O2A-CGA	2.72	1.41	1.33
14	A2	1642	CLA	O2D-CGD	2.72	1.40	1.33
14	A1	830	CLA	OBD-CAD	2.72	1.26	1.22
14	A3	821	CLA	CHB-C4A	2.72	1.36	1.33
14	B2	806	CLA	C3D-C2D	2.72	1.45	1.39
17	A2	1654	LHG	P-O6	2.72	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A4	820	CLA	CHB-C4A	2.72	1.36	1.33
14	A5	827	CLA	O2A-CGA	2.72	1.41	1.33
14	B6	816	CLA	C3D-C2D	2.72	1.45	1.39
14	B3	1830	CLA	O2D-CGD	2.72	1.40	1.33
14	A1	822	CLA	OBD-CAD	2.72	1.26	1.22
14	B6	829	CLA	C3B-C2B	2.72	1.44	1.40
14	A1	811	CLA	O2A-CGA	2.72	1.41	1.33
14	A2	1641	CLA	O2D-CGD	2.72	1.40	1.33
14	J1	102	CLA	OBD-CAD	2.72	1.26	1.22
14	A4	833	CLA	OBD-CAD	2.72	1.26	1.22
14	A6	1624	CLA	OBD-CAD	2.72	1.26	1.22
14	A3	833	CLA	CHC-C1C	2.73	1.43	1.35
14	A5	831	CLA	O2D-CGD	2.73	1.40	1.33
14	A4	827	CLA	O2D-CGD	2.73	1.40	1.33
14	B4	809	CLA	OBD-CAD	2.73	1.26	1.22
14	B1	837	CLA	O2D-CGD	2.73	1.40	1.33
14	B6	833	CLA	O2D-CGD	2.73	1.40	1.33
14	B3	1838	CLA	O2D-CGD	2.73	1.40	1.33
16	B3	1845	BCR	C26-C25	2.73	1.39	1.34
14	A4	828	CLA	C3D-C2D	2.73	1.45	1.39
14	B2	828	CLA	C3B-C2B	2.73	1.44	1.40
14	A2	1637	CLA	O2D-CGD	2.73	1.40	1.33
14	B1	836	CLA	CHB-C4A	2.73	1.36	1.33
14	A5	831	CLA	CHB-C4A	2.73	1.36	1.33
14	B2	832	CLA	O2D-CGD	2.73	1.40	1.33
14	B1	831	CLA	O2D-CGD	2.73	1.40	1.33
14	B5	1832	CLA	O2D-CGD	2.73	1.40	1.33
14	L2	206	CLA	CHB-C4A	2.73	1.36	1.33
14	A5	818	CLA	OBD-CAD	2.73	1.26	1.22
14	B3	1824	CLA	OBD-CAD	2.73	1.26	1.22
14	A2	1636	CLA	OBD-CAD	2.73	1.26	1.22
14	A6	1612	CLA	O2D-CGD	2.73	1.40	1.33
14	A2	1638	CLA	CHC-C1C	2.73	1.43	1.35
14	B2	840	CLA	OBD-CAD	2.73	1.26	1.22
14	A2	1610	CLA	O2D-CGD	2.73	1.40	1.33
14	B3	1837	CLA	CHB-C4A	2.73	1.36	1.33
14	A2	1622	CLA	O2A-CGA	2.73	1.41	1.33
14	B6	824	CLA	O2D-CGD	2.73	1.40	1.33
14	A2	1632	CLA	OBD-CAD	2.73	1.26	1.22
14	A1	829	CLA	OBD-CAD	2.73	1.26	1.22
14	A4	826	CLA	O2A-CGA	2.74	1.41	1.33
14	B1	836	CLA	O2D-CGD	2.74	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L3	201	BCR	C30-C25	2.74	1.57	1.53
14	L2	202	CLA	O2D-CGD	2.74	1.40	1.33
14	A4	812	CLA	O2D-CGD	2.74	1.40	1.33
14	B3	1818	CLA	C3D-C2D	2.74	1.45	1.39
14	B3	1811	CLA	CHC-C1C	2.74	1.43	1.35
14	A6	1615	CLA	O2D-CGD	2.74	1.40	1.33
19	B5	1851	LMG	O7-C10	2.74	1.42	1.34
14	A3	834	CLA	O2D-CGD	2.74	1.40	1.33
14	B3	1834	CLA	CHB-C4A	2.74	1.36	1.33
14	A2	1630	CLA	O2D-CGD	2.74	1.40	1.33
14	A3	805	CLA	O2D-CGD	2.74	1.40	1.33
14	B2	804	CLA	OBD-CAD	2.74	1.26	1.22
14	B1	832	CLA	O2D-CGD	2.74	1.40	1.33
14	A4	807	CLA	O2D-CGD	2.74	1.40	1.33
14	B6	833	CLA	OBD-CAD	2.74	1.26	1.22
14	B3	1818	CLA	O2A-CGA	2.74	1.41	1.33
14	A5	825	CLA	O2D-CGD	2.75	1.40	1.33
14	A6	1636	CLA	CHC-C1C	2.75	1.43	1.35
14	A1	830	CLA	O2D-CGD	2.75	1.40	1.33
14	B4	815	CLA	O2D-CGD	2.75	1.40	1.33
14	A1	830	CLA	CHB-C4A	2.75	1.36	1.33
14	A5	803	CLA	OBD-CAD	2.75	1.26	1.22
14	A5	817	CLA	OBD-CAD	2.75	1.26	1.22
14	B3	1819	CLA	CHB-C4A	2.75	1.36	1.33
14	B1	831	CLA	OBD-CAD	2.75	1.26	1.22
14	A1	820	CLA	CHB-C4A	2.75	1.36	1.33
14	A3	844	CLA	OBD-CAD	2.75	1.26	1.22
14	A2	1614	CLA	O2A-CGA	2.75	1.41	1.33
14	A6	1620	CLA	O2A-CGA	2.75	1.41	1.33
14	J6	1103	CLA	OBD-CAD	2.75	1.26	1.22
14	B1	826	CLA	OBD-CAD	2.75	1.26	1.22
14	A2	1615	CLA	O2D-CGD	2.75	1.40	1.33
14	A3	836	CLA	O2D-CGD	2.75	1.40	1.33
14	A5	820	CLA	O2A-CGA	2.75	1.41	1.33
14	A5	812	CLA	O2D-CGD	2.75	1.40	1.33
14	A6	1629	CLA	OBD-CAD	2.75	1.26	1.22
14	B2	812	CLA	O2D-CGD	2.76	1.40	1.33
14	A3	814	CLA	CHB-C4A	2.76	1.36	1.33
14	B6	814	CLA	O2D-CGD	2.76	1.40	1.33
14	B5	1803	CLA	C3D-C2D	2.76	1.45	1.39
16	F4	204	BCR	C30-C25	2.76	1.57	1.53
14	B1	817	CLA	O2A-CGA	2.76	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L1	201	CLA	O2A-CGA	2.76	1.41	1.33
14	A4	822	CLA	O2A-CGA	2.76	1.41	1.33
14	A5	832	CLA	O2A-CGA	2.76	1.41	1.33
14	A3	813	CLA	OBD-CAD	2.76	1.26	1.22
14	B1	812	CLA	O2D-CGD	2.76	1.40	1.33
14	A5	834	CLA	OBD-CAD	2.76	1.26	1.22
14	A5	815	CLA	O2D-CGD	2.76	1.40	1.33
14	A6	1625	CLA	OBD-CAD	2.76	1.26	1.22
14	L4	204	CLA	CHB-C4A	2.76	1.36	1.33
14	J2	101	CLA	O2D-CGD	2.76	1.40	1.33
14	A1	832	CLA	OBD-CAD	2.76	1.26	1.22
14	B4	823	CLA	O2D-CGD	2.76	1.40	1.33
14	B2	817	CLA	O2D-CGD	2.76	1.40	1.33
14	B5	1835	CLA	O2D-CGD	2.76	1.40	1.33
14	L6	202	CLA	O2A-CGA	2.76	1.41	1.33
14	A1	812	CLA	O2D-CGD	2.76	1.40	1.33
14	A2	1629	CLA	O2A-CGA	2.76	1.41	1.33
19	B4	851	LMG	O7-C10	2.76	1.42	1.34
14	A5	828	CLA	OBD-CAD	2.77	1.26	1.22
14	A1	824	CLA	O2D-CGD	2.77	1.40	1.33
14	A6	1631	CLA	CHB-C4A	2.77	1.36	1.33
14	J6	1101	CLA	OBD-CAD	2.77	1.26	1.22
14	A4	818	CLA	C3D-C2D	2.77	1.45	1.39
14	L1	202	CLA	O2D-CGD	2.77	1.40	1.33
14	A3	810	CLA	OBD-CAD	2.77	1.26	1.22
14	B1	834	CLA	O2A-CGA	2.77	1.41	1.33
14	B4	833	CLA	O2A-CGA	2.77	1.41	1.33
14	B1	829	CLA	O2A-CGA	2.77	1.41	1.33
14	A5	829	CLA	OBD-CAD	2.77	1.26	1.22
14	A4	817	CLA	OBD-CAD	2.77	1.26	1.22
14	A1	819	CLA	O2A-CGA	2.77	1.41	1.33
14	B6	835	CLA	CHB-C4A	2.77	1.36	1.33
14	B4	852	CLA	O2D-CGD	2.77	1.40	1.33
14	B3	1809	CLA	C3D-C2D	2.77	1.45	1.39
14	B6	822	CLA	OBD-CAD	2.77	1.26	1.22
14	A3	837	CLA	CHC-C1C	2.77	1.43	1.35
14	A3	832	CLA	O2A-CGA	2.77	1.41	1.33
14	B6	816	CLA	OBD-CAD	2.77	1.26	1.22
14	B5	1826	CLA	O2D-CGD	2.77	1.40	1.33
14	A1	806	CLA	OBD-CAD	2.78	1.26	1.22
14	B4	818	CLA	O2A-CGA	2.78	1.41	1.33
14	A2	1623	CLA	O2D-CGD	2.78	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B5	1802	CLA	OBD-CAD	2.78	1.26	1.22
14	B6	820	CLA	OBD-CAD	2.78	1.26	1.22
14	B5	1830	CLA	O2A-CGA	2.78	1.41	1.33
14	B4	832	CLA	O2D-CGD	2.78	1.40	1.33
14	A2	1605	CLA	OBD-CAD	2.78	1.26	1.22
14	A6	1623	CLA	O2A-CGA	2.78	1.41	1.33
14	A1	822	CLA	O2A-CGA	2.78	1.41	1.33
14	A6	1651	CLA	C3D-C2D	2.78	1.45	1.39
14	A1	831	CLA	CHC-C1C	2.78	1.43	1.35
16	B3	1851	BCR	C30-C25	2.78	1.57	1.53
14	A2	1645	CLA	C3D-C2D	2.78	1.45	1.39
14	B3	1815	CLA	O2D-CGD	2.78	1.40	1.33
14	L4	204	CLA	OBD-CAD	2.78	1.26	1.22
14	A6	1621	CLA	O2D-CGD	2.78	1.40	1.33
14	B6	840	CLA	O2A-CGA	2.78	1.41	1.33
14	A3	833	CLA	O2D-CGD	2.78	1.40	1.33
14	A1	816	CLA	OBD-CAD	2.78	1.26	1.22
14	B5	1809	CLA	OBD-CAD	2.78	1.26	1.22
14	A3	816	CLA	O2D-CGD	2.78	1.40	1.33
14	B3	1835	CLA	O2A-CGA	2.79	1.41	1.33
14	B4	822	CLA	O2D-CGD	2.79	1.40	1.33
14	A5	821	CLA	O2D-CGD	2.79	1.40	1.33
14	B5	1822	CLA	O2D-CGD	2.79	1.40	1.33
14	J3	102	CLA	C3D-C2D	2.79	1.45	1.39
14	B5	1833	CLA	O2A-CGA	2.79	1.41	1.33
14	B5	1826	CLA	OBD-CAD	2.79	1.26	1.22
14	K5	101	CLA	C3D-C2D	2.79	1.45	1.39
14	A5	836	CLA	CHC-C1C	2.79	1.43	1.35
16	A4	844	BCR	C30-C25	2.79	1.57	1.53
14	B3	1842	CLA	O2A-CGA	2.79	1.41	1.33
14	A1	826	CLA	O2A-CGA	2.79	1.41	1.33
14	A3	803	CLA	OBD-CAD	2.79	1.26	1.22
14	A1	831	CLA	O2D-CGD	2.79	1.40	1.33
14	B6	802	CLA	C3D-C2D	2.79	1.45	1.39
14	B2	810	CLA	O2D-CGD	2.79	1.40	1.33
14	A3	812	CLA	O2D-CGD	2.79	1.40	1.33
14	B4	818	CLA	OBD-CAD	2.80	1.26	1.22
14	B6	837	CLA	C3D-C2D	2.80	1.45	1.39
17	A3	854	LHG	P-O6	2.80	1.70	1.59
16	B1	852	BCR	C30-C25	2.80	1.57	1.53
14	B6	836	CLA	O2D-CGD	2.80	1.40	1.33
14	A4	809	CLA	OBD-CAD	2.80	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B2	832	CLA	OBD-CAD	2.80	1.26	1.22
14	J3	102	CLA	OBD-CAD	2.80	1.26	1.22
14	B4	826	CLA	O2D-CGD	2.80	1.40	1.33
14	B6	833	CLA	O2A-CGA	2.80	1.41	1.33
14	B4	820	CLA	C3B-C2B	2.80	1.44	1.40
14	A3	818	CLA	OBD-CAD	2.80	1.26	1.22
14	B1	830	CLA	C3B-C2B	2.80	1.44	1.40
14	A4	814	CLA	O2D-CGD	2.80	1.40	1.33
14	B2	810	CLA	OBD-CAD	2.80	1.26	1.22
14	A2	1607	CLA	O2D-CGD	2.80	1.40	1.33
14	B1	834	CLA	O2D-CGD	2.80	1.40	1.33
14	A2	1603	CLA	C3D-C2D	2.80	1.45	1.39
14	B3	1814	CLA	OBD-CAD	2.80	1.26	1.22
14	B2	823	CLA	O2D-CGD	2.80	1.40	1.33
14	B2	821	CLA	O2A-CGA	2.80	1.41	1.33
14	A3	823	CLA	O2A-CGA	2.80	1.41	1.33
14	A6	1607	CLA	OBD-CAD	2.80	1.26	1.22
14	B1	825	CLA	O2D-CGD	2.81	1.40	1.33
14	A2	1616	CLA	CHB-C4A	2.81	1.36	1.33
14	B6	821	CLA	O2D-CGD	2.81	1.40	1.33
14	F2	202	CLA	C3D-C2D	2.81	1.45	1.39
14	A1	813	CLA	C3D-C2D	2.81	1.45	1.39
14	B6	841	CLA	OBD-CAD	2.81	1.26	1.22
14	A1	813	CLA	CHB-C4A	2.81	1.36	1.33
14	B5	1813	CLA	O2D-CGD	2.81	1.40	1.33
14	B1	829	CLA	OBD-CAD	2.81	1.26	1.22
16	L5	207	BCR	C30-C25	2.81	1.57	1.53
14	B6	830	CLA	OBD-CAD	2.81	1.26	1.22
14	B2	832	CLA	O2A-CGA	2.81	1.41	1.33
14	A6	1626	CLA	CHB-C4A	2.81	1.36	1.33
19	B1	850	LMG	O7-C10	2.81	1.42	1.34
14	A6	1617	CLA	OBD-CAD	2.81	1.26	1.22
14	B2	816	CLA	OBD-CAD	2.81	1.26	1.22
14	A2	1617	CLA	O2D-CGD	2.81	1.40	1.33
14	B2	821	CLA	OBD-CAD	2.81	1.26	1.22
14	J3	101	CLA	O2D-CGD	2.81	1.40	1.33
14	L4	201	CLA	O2D-CGD	2.81	1.40	1.33
14	A5	810	CLA	OBD-CAD	2.81	1.26	1.22
14	A5	842	CLA	CHC-C1C	2.81	1.43	1.35
14	A4	820	CLA	O2D-CGD	2.81	1.40	1.33
14	A6	1633	CLA	O2D-CGD	2.81	1.40	1.33
14	B2	810	CLA	CHB-C4A	2.81	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B3	1823	CLA	O2D-CGD	2.82	1.40	1.33
14	B1	804	CLA	OBD-CAD	2.82	1.26	1.22
14	B5	1818	CLA	O2A-CGA	2.82	1.41	1.33
14	I1	101	CLA	CHC-C1C	2.82	1.43	1.35
14	B1	803	CLA	OBD-CAD	2.82	1.26	1.22
14	B3	1833	CLA	O2A-CGA	2.82	1.41	1.33
14	A6	1616	CLA	O2D-CGD	2.82	1.40	1.33
14	A4	829	CLA	OBD-CAD	2.82	1.26	1.22
14	A1	804	CLA	O2D-CGD	2.82	1.40	1.33
14	B6	831	CLA	O2A-CGA	2.82	1.41	1.33
14	B6	838	CLA	O2D-CGD	2.82	1.40	1.33
14	A5	805	CLA	O2D-CGD	2.82	1.40	1.33
14	A3	814	CLA	OBD-CAD	2.82	1.26	1.22
14	A6	1620	CLA	OBD-CAD	2.82	1.26	1.22
14	B2	836	CLA	C3D-C2D	2.82	1.45	1.39
14	A5	843	CLA	O2D-CGD	2.82	1.40	1.33
14	B1	832	CLA	O2A-CGA	2.82	1.41	1.33
14	A5	837	CLA	CHB-C4A	2.82	1.36	1.33
14	A3	835	CLA	O2D-CGD	2.82	1.40	1.33
14	B4	811	CLA	CHC-C1C	2.82	1.43	1.35
14	B4	842	CLA	CHC-C1C	2.82	1.43	1.35
14	J1	101	CLA	O2D-CGD	2.82	1.40	1.33
17	A6	1650	LHG	P-O6	2.82	1.70	1.59
14	A6	1627	CLA	O2A-CGA	2.83	1.41	1.33
14	B3	1813	CLA	O2D-CGD	2.83	1.40	1.33
14	A2	1641	CLA	OBD-CAD	2.83	1.26	1.22
14	B2	827	CLA	O2A-CGA	2.83	1.41	1.33
14	B1	853	CLA	O2D-CGD	2.83	1.40	1.33
14	B3	1826	CLA	O2D-CGD	2.83	1.40	1.33
14	B4	830	CLA	O2A-CGA	2.83	1.41	1.33
14	B2	815	CLA	O2A-CGA	2.83	1.41	1.33
14	A6	1637	CLA	CHB-C4A	2.83	1.36	1.33
14	A2	1639	CLA	CHB-C4A	2.83	1.36	1.33
14	B4	835	CLA	OBD-CAD	2.83	1.26	1.22
14	A3	821	CLA	O2D-CGD	2.83	1.40	1.33
14	B4	803	CLA	OBD-CAD	2.83	1.26	1.22
14	A6	1604	CLA	OBD-CAD	2.83	1.26	1.22
14	B1	838	CLA	C3D-C2D	2.83	1.45	1.39
14	A5	802	CLA	C3D-C2D	2.83	1.45	1.39
14	B2	808	CLA	OBD-CAD	2.83	1.26	1.22
14	A5	833	CLA	O2D-CGD	2.83	1.40	1.33
14	B4	826	CLA	OBD-CAD	2.83	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A4	828	CLA	OBD-CAD	2.83	1.26	1.22
14	A6	1622	CLA	O2D-CGD	2.83	1.40	1.33
14	A4	802	CLA	OBD-CAD	2.84	1.26	1.22
14	B2	820	CLA	OBD-CAD	2.84	1.26	1.22
14	B3	1830	CLA	CHB-C4A	2.84	1.36	1.33
14	A2	1616	CLA	O2D-CGD	2.84	1.40	1.33
16	A3	850	BCR	C30-C25	2.84	1.57	1.53
14	B4	816	CLA	OBD-CAD	2.84	1.26	1.22
14	L5	203	CLA	O2D-CGD	2.84	1.40	1.33
14	J4	102	CLA	C3D-C2D	2.84	1.45	1.39
14	B1	802	CLA	OBD-CAD	2.84	1.26	1.22
14	B2	834	CLA	CHB-C4A	2.84	1.36	1.33
14	B5	1843	CLA	OBD-CAD	2.84	1.26	1.22
14	J4	101	CLA	O2D-CGD	2.84	1.40	1.33
14	A6	1621	CLA	CHB-C4A	2.84	1.36	1.33
14	B2	802	CLA	C3D-C2D	2.84	1.45	1.39
14	A1	811	CLA	O2D-CGD	2.84	1.40	1.33
14	A5	817	CLA	O2A-CGA	2.84	1.41	1.33
14	B6	824	CLA	O2A-CGA	2.84	1.41	1.33
14	B3	1824	CLA	O2D-CGD	2.84	1.40	1.33
14	A6	1603	CLA	OBD-CAD	2.84	1.26	1.22
14	A4	830	CLA	CHB-C4A	2.84	1.36	1.33
14	B3	1813	CLA	OBD-CAD	2.84	1.26	1.22
14	B6	804	CLA	OBD-CAD	2.84	1.26	1.22
14	B3	1830	CLA	O2A-CGA	2.85	1.41	1.33
14	B4	824	CLA	O2A-CGA	2.85	1.41	1.33
14	B6	828	CLA	O2A-CGA	2.85	1.41	1.33
14	B4	843	CLA	OBD-CAD	2.85	1.26	1.22
14	A4	832	CLA	O2D-CGD	2.85	1.40	1.33
14	B2	829	CLA	O2D-CGD	2.85	1.40	1.33
14	B2	823	CLA	O2A-CGA	2.85	1.41	1.33
14	B5	1824	CLA	O2D-CGD	2.85	1.40	1.33
14	B3	1835	CLA	OBD-CAD	2.85	1.26	1.22
14	B5	1832	CLA	OBD-CAD	2.85	1.26	1.22
14	L3	204	CLA	CHB-C4A	2.85	1.36	1.33
14	B4	802	CLA	OBD-CAD	2.85	1.26	1.22
14	F2	204	CLA	C3D-C2D	2.85	1.45	1.39
14	B1	811	CLA	CHC-C1C	2.85	1.43	1.35
14	A1	839	CLA	CHC-C1C	2.85	1.43	1.35
14	A2	1624	CLA	O2D-CGD	2.85	1.40	1.33
17	A5	852	LHG	P-O6	2.85	1.70	1.59
14	A6	1619	CLA	CHC-C1C	2.85	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B4	813	CLA	O2D-CGD	2.85	1.40	1.33
14	B6	816	CLA	O2A-CGA	2.85	1.41	1.33
14	B6	813	CLA	OBD-CAD	2.85	1.26	1.22
16	L1	209	BCR	C30-C25	2.85	1.57	1.53
14	B3	1827	CLA	OBD-CAD	2.85	1.26	1.22
14	A1	818	CLA	C3D-C2D	2.85	1.45	1.39
14	L2	207	CLA	CHB-C4A	2.85	1.36	1.33
14	A6	1623	CLA	OBD-CAD	2.86	1.26	1.22
14	A2	1615	CLA	OBD-CAD	2.86	1.26	1.22
14	A1	833	CLA	OBD-CAD	2.86	1.26	1.22
14	B2	819	CLA	OBD-CAD	2.86	1.26	1.22
14	B1	805	CLA	C3D-C2D	2.86	1.45	1.39
14	A3	814	CLA	O2D-CGD	2.86	1.40	1.33
14	A5	807	CLA	OBD-CAD	2.86	1.26	1.22
14	A3	843	CLA	CHC-C1C	2.86	1.43	1.35
19	B6	848	LMG	O7-C10	2.86	1.42	1.34
14	B1	833	CLA	CHB-C4A	2.86	1.36	1.33
14	B5	1839	CLA	OBD-CAD	2.86	1.26	1.22
14	A6	1610	CLA	OBD-CAD	2.86	1.26	1.22
14	B2	821	CLA	O2D-CGD	2.86	1.40	1.33
14	A1	814	CLA	O2D-CGD	2.86	1.40	1.33
14	B5	1835	CLA	O2A-CGA	2.86	1.41	1.33
14	B2	801	CLA	OBD-CAD	2.86	1.26	1.22
14	A6	1634	CLA	OBD-CAD	2.86	1.26	1.22
14	L6	203	CLA	CHC-C1C	2.86	1.43	1.35
14	B2	812	CLA	OBD-CAD	2.86	1.26	1.22
14	A2	1635	CLA	O2D-CGD	2.86	1.40	1.33
14	A2	1634	CLA	CHC-C1C	2.86	1.43	1.35
14	B6	811	CLA	OBD-CAD	2.86	1.26	1.22
14	B3	1832	CLA	O2D-CGD	2.86	1.40	1.33
14	A3	838	CLA	CHB-C4A	2.86	1.36	1.33
16	B6	850	BCR	C30-C25	2.86	1.57	1.53
14	B5	1824	CLA	O2A-CGA	2.86	1.41	1.33
14	B3	1826	CLA	O2A-CGA	2.86	1.41	1.33
14	B2	819	CLA	O2D-CGD	2.87	1.40	1.33
17	A1	849	LHG	P-O6	2.87	1.70	1.59
14	A4	807	CLA	OBD-CAD	2.87	1.26	1.22
14	A5	814	CLA	CHB-C4A	2.87	1.36	1.33
14	B1	828	CLA	CHB-C4A	2.87	1.36	1.33
16	J5	105	BCR	C30-C25	2.87	1.57	1.53
14	A2	1633	CLA	CHB-C4A	2.87	1.36	1.33
14	B2	820	CLA	O2D-CGD	2.87	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A4	824	CLA	OBD-CAD	2.87	1.26	1.22
14	B3	1801	CLA	CHB-C4A	2.87	1.36	1.33
14	B1	829	CLA	CHB-C4A	2.87	1.36	1.33
14	J5	102	CLA	C3D-C2D	2.87	1.45	1.39
14	B4	809	CLA	C3D-C2D	2.87	1.45	1.39
14	B6	822	CLA	O2D-CGD	2.87	1.40	1.33
14	B1	817	CLA	OBD-CAD	2.87	1.26	1.22
14	A1	819	CLA	OBD-CAD	2.87	1.26	1.22
14	B5	1842	CLA	CHC-C1C	2.87	1.43	1.35
14	B2	830	CLA	O2A-CGA	2.87	1.41	1.33
14	A1	840	CLA	C3D-C2D	2.87	1.45	1.39
14	A3	840	CLA	CHB-C4A	2.87	1.36	1.33
14	B1	853	CLA	CHB-C4A	2.87	1.36	1.33
14	A6	1632	CLA	O2D-CGD	2.87	1.40	1.33
14	B2	826	CLA	CHB-C4A	2.88	1.36	1.33
14	A5	808	CLA	OBD-CAD	2.88	1.26	1.22
14	B2	808	CLA	CHC-C1C	2.88	1.43	1.35
14	B3	1804	CLA	C3D-C2D	2.88	1.45	1.39
19	B2	848	LMG	O7-C10	2.88	1.42	1.34
14	A6	1614	CLA	CHB-C4A	2.88	1.36	1.33
14	A3	835	CLA	OBD-CAD	2.88	1.26	1.22
14	A4	831	CLA	CHC-C1C	2.88	1.43	1.35
14	J6	1103	CLA	C3D-C2D	2.88	1.45	1.39
14	B1	812	CLA	OBD-CAD	2.88	1.26	1.22
14	B5	1814	CLA	OBD-CAD	2.88	1.26	1.22
14	A1	834	CLA	CHC-C1C	2.88	1.43	1.35
14	B3	1822	CLA	O2D-CGD	2.88	1.40	1.33
14	A5	843	CLA	CHB-C4A	2.88	1.36	1.33
14	B1	823	CLA	O2D-CGD	2.88	1.40	1.33
14	A4	816	CLA	OBD-CAD	2.88	1.26	1.22
14	A1	812	CLA	OBD-CAD	2.88	1.26	1.22
14	B2	815	CLA	OBD-CAD	2.88	1.26	1.22
14	B3	1801	CLA	O2D-CGD	2.88	1.40	1.33
14	A4	835	CLA	CHC-C1C	2.89	1.43	1.35
14	B5	1804	CLA	C3D-C2D	2.89	1.45	1.39
14	B2	812	CLA	CHB-C4A	2.89	1.36	1.33
14	B3	1843	CLA	OBD-CAD	2.89	1.26	1.22
14	A1	816	CLA	O2A-CGA	2.89	1.41	1.33
14	B5	1803	CLA	OBD-CAD	2.89	1.26	1.22
14	A6	1613	CLA	OBD-CAD	2.89	1.26	1.22
14	A5	816	CLA	O2D-CGD	2.89	1.40	1.33
14	A3	802	CLA	C3D-C2D	2.89	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B6	830	CLA	O2D-CGD	2.89	1.40	1.33
14	B6	828	CLA	CHB-C4A	2.89	1.36	1.33
14	B4	832	CLA	OBD-CAD	2.89	1.26	1.22
14	B1	801	CLA	C3D-C2D	2.89	1.45	1.39
14	J5	101	CLA	O2D-CGD	2.89	1.40	1.33
14	A3	825	CLA	OBD-CAD	2.89	1.26	1.22
14	B6	820	CLA	O2D-CGD	2.89	1.40	1.33
14	B1	821	CLA	O2D-CGD	2.89	1.40	1.33
14	B4	826	CLA	O2A-CGA	2.89	1.41	1.33
14	L6	202	CLA	CHC-C1C	2.89	1.43	1.35
14	B3	1824	CLA	O2A-CGA	2.89	1.41	1.33
14	A4	841	CLA	CHC-C1C	2.90	1.43	1.35
16	L6	201	BCR	C30-C25	2.90	1.57	1.53
14	B3	1830	CLA	OBD-CAD	2.90	1.26	1.22
14	B4	840	CLA	OBD-CAD	2.90	1.26	1.22
14	B6	806	CLA	OBD-CAD	2.90	1.26	1.22
17	A3	853	LHG	P-O3	2.90	1.71	1.59
14	B3	1840	CLA	O2D-CGD	2.90	1.40	1.33
14	B3	1839	CLA	OBD-CAD	2.90	1.26	1.22
14	B1	822	CLA	O2D-CGD	2.90	1.40	1.33
14	B3	1842	CLA	CHC-C1C	2.90	1.43	1.35
14	B4	804	CLA	C3D-C2D	2.90	1.45	1.39
14	A1	802	CLA	OBD-CAD	2.90	1.26	1.22
14	B5	1815	CLA	CHB-C4A	2.90	1.36	1.33
14	A2	1614	CLA	O2D-CGD	2.90	1.40	1.33
14	A2	1644	CLA	CHC-C1C	2.90	1.43	1.35
14	A5	813	CLA	OBD-CAD	2.90	1.26	1.22
14	B4	801	CLA	C3D-C2D	2.91	1.45	1.39
14	B3	1839	CLA	C3D-C2D	2.91	1.45	1.39
14	A1	802	CLA	CHB-C4A	2.91	1.36	1.33
14	A3	817	CLA	OBD-CAD	2.91	1.26	1.22
14	A3	822	CLA	O2D-CGD	2.91	1.40	1.33
14	B5	1829	CLA	CHB-C4A	2.91	1.36	1.33
14	B2	827	CLA	OBD-CAD	2.91	1.26	1.22
14	B4	835	CLA	O2A-CGA	2.91	1.41	1.33
14	A4	804	CLA	O2D-CGD	2.91	1.40	1.33
14	B3	1818	CLA	OBD-CAD	2.91	1.26	1.22
14	A1	835	CLA	CHB-C4A	2.91	1.36	1.33
14	B3	1809	CLA	OBD-CAD	2.91	1.26	1.22
14	A4	812	CLA	OBD-CAD	2.91	1.26	1.22
14	A6	1639	CLA	CHC-C1C	2.91	1.43	1.35
14	A5	822	CLA	O2D-CGD	2.91	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	832	CLA	CHC-C1C	2.91	1.43	1.35
19	B3	1850	LMG	O7-C10	2.91	1.42	1.34
14	L1	201	CLA	CHC-C1C	2.91	1.43	1.35
14	B3	1840	CLA	OBD-CAD	2.91	1.26	1.22
14	A2	1622	CLA	OBD-CAD	2.91	1.26	1.22
14	A1	809	CLA	OBD-CAD	2.92	1.26	1.22
14	B4	824	CLA	OBD-CAD	2.92	1.26	1.22
14	A6	1605	CLA	O2D-CGD	2.92	1.40	1.33
14	A4	813	CLA	CHB-C4A	2.92	1.36	1.33
14	B6	803	CLA	CHB-C4A	2.92	1.36	1.33
14	A6	1617	CLA	O2A-CGA	2.92	1.41	1.33
14	B1	841	CLA	OBD-CAD	2.92	1.26	1.22
14	A3	819	CLA	CHC-C1C	2.92	1.43	1.35
16	L4	208	BCR	C30-C25	2.92	1.57	1.53
14	A3	832	CLA	CHC-C1C	2.92	1.43	1.35
14	A1	821	CLA	O2D-CGD	2.92	1.40	1.33
14	A3	843	CLA	CHB-C4A	2.92	1.36	1.33
14	B6	821	CLA	OBD-CAD	2.92	1.26	1.22
14	B2	839	CLA	CHC-C1C	2.92	1.43	1.35
16	I1	103	BCR	C30-C25	2.92	1.57	1.53
14	B5	1801	CLA	CHB-C4A	2.92	1.36	1.33
16	L3	206	BCR	C30-C25	2.92	1.57	1.53
14	X5	101	CLA	OBD-CAD	2.92	1.26	1.22
14	B6	822	CLA	O2A-CGA	2.92	1.41	1.33
14	B4	824	CLA	O2D-CGD	2.92	1.40	1.33
14	A4	822	CLA	OBD-CAD	2.92	1.26	1.22
14	A3	806	CLA	O2D-CGD	2.92	1.40	1.33
14	A3	841	CLA	OBD-CAD	2.93	1.26	1.22
14	B4	839	CLA	OBD-CAD	2.93	1.26	1.22
14	A5	825	CLA	OBD-CAD	2.93	1.26	1.22
14	A3	845	CLA	O2D-CGD	2.93	1.40	1.33
16	A5	848	BCR	C30-C25	2.93	1.57	1.53
14	A6	1635	CLA	OBD-CAD	2.93	1.26	1.22
14	A4	815	CLA	O2D-CGD	2.93	1.40	1.33
14	A4	821	CLA	O2D-CGD	2.93	1.40	1.33
14	B3	1837	CLA	OBD-CAD	2.93	1.26	1.22
14	A6	1614	CLA	O2D-CGD	2.93	1.40	1.33
14	B5	1818	CLA	OBD-CAD	2.93	1.26	1.22
14	B3	1816	CLA	OBD-CAD	2.93	1.26	1.22
14	A2	1612	CLA	OBD-CAD	2.93	1.26	1.22
14	J1	102	CLA	C3D-C2D	2.93	1.45	1.39
14	B4	829	CLA	CHB-C4A	2.94	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B5	1830	CLA	CHB-C4A	2.94	1.36	1.33
14	B6	840	CLA	CHC-C1C	2.94	1.43	1.35
14	A1	827	CLA	CHC-C1C	2.94	1.43	1.35
14	A4	838	CLA	OBD-CAD	2.94	1.26	1.22
14	A2	1604	CLA	OBD-CAD	2.94	1.26	1.22
14	A2	1618	CLA	O2D-CGD	2.94	1.40	1.33
14	A2	1619	CLA	O2A-CGA	2.94	1.41	1.33
14	B5	1813	CLA	OBD-CAD	2.94	1.26	1.22
14	B4	822	CLA	OBD-CAD	2.94	1.26	1.22
14	B6	813	CLA	O2D-CGD	2.94	1.40	1.33
17	A2	1653	LHG	P-O3	2.94	1.71	1.59
14	A1	824	CLA	OBD-CAD	2.94	1.26	1.22
14	A6	1612	CLA	OBD-CAD	2.94	1.26	1.22
14	A2	1627	CLA	OBD-CAD	2.94	1.26	1.22
14	A5	803	CLA	CHB-C4A	2.94	1.37	1.33
14	B5	1840	CLA	O2D-CGD	2.94	1.40	1.33
14	B6	828	CLA	OBD-CAD	2.94	1.26	1.22
14	B4	830	CLA	OBD-CAD	2.95	1.26	1.22
14	B6	817	CLA	OBD-CAD	2.95	1.26	1.22
14	A3	817	CLA	O2A-CGA	2.95	1.41	1.33
14	A4	819	CLA	OBD-CAD	2.95	1.26	1.22
14	A3	836	CLA	OBD-CAD	2.95	1.26	1.22
14	A2	1642	CLA	O2A-CGA	2.95	1.41	1.33
14	A4	811	CLA	O2D-CGD	2.95	1.40	1.33
14	B2	814	CLA	CHB-C4A	2.95	1.37	1.33
14	B1	823	CLA	O2A-CGA	2.95	1.41	1.33
14	B5	1813	CLA	CHB-C4A	2.95	1.37	1.33
14	A2	1609	CLA	OBD-CAD	2.95	1.26	1.22
14	B4	827	CLA	OBD-CAD	2.95	1.26	1.22
14	A3	807	CLA	OBD-CAD	2.95	1.26	1.22
14	L2	206	CLA	OBD-CAD	2.96	1.26	1.22
14	B3	1832	CLA	OBD-CAD	2.96	1.26	1.22
14	A5	814	CLA	O2D-CGD	2.96	1.40	1.33
14	A2	1621	CLA	CHC-C1C	2.96	1.43	1.35
14	A6	1639	CLA	O2A-CGA	2.96	1.41	1.33
14	B5	1823	CLA	O2D-CGD	2.96	1.40	1.33
14	B6	813	CLA	CHB-C4A	2.96	1.37	1.33
14	B3	1804	CLA	CHB-C4A	2.96	1.37	1.33
14	A2	1637	CLA	OBD-CAD	2.96	1.26	1.22
16	L6	209	BCR	C30-C25	2.96	1.57	1.53
14	B2	804	CLA	CHC-C1C	2.96	1.43	1.35
14	A1	820	CLA	O2D-CGD	2.96	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	823	CLA	OBD-CAD	2.96	1.26	1.22
16	L2	201	BCR	C30-C25	2.96	1.57	1.53
14	A5	835	CLA	OBD-CAD	2.96	1.26	1.22
14	A5	820	CLA	OBD-CAD	2.96	1.26	1.22
14	A2	1608	CLA	O2D-CGD	2.97	1.40	1.33
14	L4	205	CLA	CHB-C4A	2.97	1.37	1.33
17	A6	1649	LHG	P-O3	2.97	1.71	1.59
14	B5	1825	CLA	OBD-CAD	2.97	1.26	1.22
14	B2	834	CLA	OBD-CAD	2.97	1.26	1.22
14	B4	813	CLA	CHB-C4A	2.97	1.37	1.33
16	A4	847	BCR	C30-C25	2.97	1.57	1.53
14	J1	101	CLA	C3D-C2D	2.97	1.45	1.39
14	B4	830	CLA	CHB-C4A	2.97	1.37	1.33
14	B3	1817	CLA	CHB-C4A	2.97	1.37	1.33
14	B5	1826	CLA	O2A-CGA	2.97	1.41	1.33
14	A4	816	CLA	O2A-CGA	2.97	1.41	1.33
14	A6	1608	CLA	OBD-CAD	2.97	1.26	1.22
14	A3	826	CLA	CHB-C4A	2.98	1.37	1.33
14	A3	841	CLA	CHC-C1C	2.98	1.43	1.35
14	A4	813	CLA	O2D-CGD	2.98	1.40	1.33
14	A6	1603	CLA	CHB-C4A	2.98	1.37	1.33
14	B2	817	CLA	CHB-C4A	2.98	1.37	1.33
14	A5	840	CLA	CHC-C1C	2.98	1.43	1.35
14	B1	825	CLA	O2A-CGA	2.98	1.42	1.33
14	B1	816	CLA	CHB-C4A	2.98	1.37	1.33
17	A4	851	LHG	P-O6	2.98	1.71	1.59
14	B1	839	CLA	OBD-CAD	2.98	1.26	1.22
14	A5	840	CLA	O2A-CGA	2.98	1.42	1.33
14	L6	208	CLA	CHB-C4A	2.98	1.37	1.33
14	A5	819	CLA	CHC-C1C	2.98	1.43	1.35
14	A3	840	CLA	OBD-CAD	2.98	1.26	1.22
14	A4	839	CLA	CHC-C1C	2.98	1.43	1.35
14	L2	202	CLA	CHC-C1C	2.99	1.43	1.35
14	B2	837	CLA	O2D-CGD	2.99	1.40	1.33
14	A6	1651	CLA	CHB-C4A	2.99	1.37	1.33
14	A2	1625	CLA	OBD-CAD	2.99	1.26	1.22
14	A4	806	CLA	OBD-CAD	2.99	1.26	1.22
14	B4	852	CLA	CHB-C4A	2.99	1.37	1.33
14	A2	1642	CLA	CHC-C1C	2.99	1.43	1.35
14	B1	812	CLA	CHB-C4A	2.99	1.37	1.33
14	B4	825	CLA	OBD-CAD	2.99	1.26	1.22
14	B2	824	CLA	OBD-CAD	3.00	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L4	206	BCR	C30-C25	3.00	1.57	1.53
17	A5	851	LHG	P-O3	3.00	1.71	1.59
14	B6	803	CLA	OBD-CAD	3.00	1.26	1.22
14	A6	1633	CLA	CHC-C1C	3.00	1.43	1.35
14	B4	814	CLA	OBD-CAD	3.00	1.26	1.22
14	A3	834	CLA	CHC-C1C	3.00	1.43	1.35
14	A4	818	CLA	CHC-C1C	3.00	1.43	1.35
14	B2	840	CLA	CHC-C1C	3.00	1.43	1.35
14	L6	203	CLA	CHB-C4A	3.00	1.37	1.33
14	A6	1606	CLA	OBD-CAD	3.00	1.26	1.22
14	B5	1830	CLA	OBD-CAD	3.00	1.26	1.22
14	B1	814	CLA	CHB-C4A	3.00	1.37	1.33
14	B4	807	CLA	CHC-C1C	3.00	1.43	1.35
14	B3	1802	CLA	OBD-CAD	3.00	1.26	1.22
14	B3	1813	CLA	CHB-C4A	3.00	1.37	1.33
14	A3	845	CLA	CHB-C4A	3.00	1.37	1.33
14	A6	1606	CLA	O2D-CGD	3.01	1.40	1.33
14	B5	1822	CLA	OBD-CAD	3.01	1.26	1.22
14	A5	806	CLA	OBD-CAD	3.01	1.26	1.22
14	L5	203	CLA	CHC-C1C	3.01	1.43	1.35
14	M1	1201	CLA	O2A-CGA	3.01	1.42	1.33
14	B6	835	CLA	OBD-CAD	3.01	1.26	1.22
14	A6	1639	CLA	OBD-CAD	3.01	1.26	1.22
14	A5	806	CLA	O2D-CGD	3.01	1.40	1.33
14	B1	813	CLA	OBD-CAD	3.01	1.26	1.22
14	B2	839	CLA	CHB-C4A	3.01	1.37	1.33
14	A2	1628	CLA	CHB-C4A	3.01	1.37	1.33
16	A1	842	BCR	C30-C25	3.01	1.57	1.53
14	X3	102	CLA	OBD-CAD	3.01	1.26	1.22
14	B4	813	CLA	OBD-CAD	3.01	1.26	1.22
14	B2	801	CLA	CHC-C1C	3.01	1.43	1.35
14	B3	1806	CLA	O2A-CGA	3.01	1.42	1.33
14	X1	1701	CLA	OBD-CAD	3.01	1.26	1.22
14	A2	1630	CLA	CHC-C1C	3.01	1.43	1.35
14	B1	834	CLA	OBD-CAD	3.02	1.26	1.22
14	B5	1801	CLA	O2D-CGD	3.02	1.40	1.33
14	B1	803	CLA	CHB-C4A	3.02	1.37	1.33
14	A5	837	CLA	OBD-CAD	3.02	1.26	1.22
14	B3	1836	CLA	OBD-CAD	3.02	1.26	1.22
14	A6	1628	CLA	CHC-C1C	3.02	1.43	1.35
14	A5	828	CLA	CHC-C1C	3.02	1.43	1.35
14	B6	812	CLA	OBD-CAD	3.02	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L2	208	BCR	C30-C25	3.02	1.57	1.53
14	A6	1616	CLA	OBD-CAD	3.02	1.26	1.22
14	B1	807	CLA	OBD-CAD	3.02	1.26	1.22
14	B1	810	CLA	OBD-CAD	3.02	1.26	1.22
14	A3	841	CLA	O2A-CGA	3.02	1.42	1.33
14	A3	811	CLA	OBD-CAD	3.02	1.26	1.22
14	B3	1807	CLA	CHC-C1C	3.02	1.43	1.35
14	A1	825	CLA	CHB-C4A	3.02	1.37	1.33
14	A4	853	CLA	OBD-CAD	3.02	1.26	1.22
14	A5	812	CLA	OBD-CAD	3.02	1.26	1.22
14	A6	1614	CLA	OBD-CAD	3.02	1.26	1.22
14	B5	1840	CLA	OBD-CAD	3.03	1.26	1.22
17	A4	850	LHG	P-O3	3.03	1.71	1.59
17	X5	102	LHG	P-O3	3.03	1.71	1.59
14	B1	839	CLA	O2D-CGD	3.03	1.40	1.33
14	A4	836	CLA	CHB-C4A	3.03	1.37	1.33
14	A5	839	CLA	CHB-C4A	3.03	1.37	1.33
14	B3	1815	CLA	CHB-C4A	3.03	1.37	1.33
14	A4	825	CLA	CHB-C4A	3.03	1.37	1.33
14	A5	839	CLA	OBD-CAD	3.03	1.26	1.22
14	B4	815	CLA	CHB-C4A	3.03	1.37	1.33
14	B5	1803	CLA	CHC-C1C	3.03	1.43	1.35
14	B6	841	CLA	CHC-C1C	3.03	1.43	1.35
14	B2	811	CLA	OBD-CAD	3.03	1.26	1.22
14	A3	806	CLA	OBD-CAD	3.03	1.26	1.22
14	L1	202	CLA	CHC-C1C	3.03	1.43	1.35
14	B1	808	CLA	CHC-C1C	3.03	1.43	1.35
14	A1	837	CLA	CHC-C1C	3.03	1.43	1.35
14	B4	840	CLA	O2D-CGD	3.03	1.40	1.33
14	A2	1613	CLA	OBD-CAD	3.03	1.26	1.22
17	B1	851	LHG	P-O3	3.03	1.71	1.59
14	A3	816	CLA	OBD-CAD	3.04	1.26	1.22
14	L4	201	CLA	CHC-C1C	3.04	1.43	1.35
14	B6	815	CLA	CHB-C4A	3.04	1.37	1.33
14	B4	843	CLA	CHC-C1C	3.04	1.43	1.35
14	A5	815	CLA	OBD-CAD	3.04	1.26	1.22
14	A3	808	CLA	OBD-CAD	3.04	1.26	1.22
14	B5	1842	CLA	CHB-C4A	3.04	1.37	1.33
14	A4	821	CLA	OBD-CAD	3.04	1.26	1.22
14	A1	818	CLA	CHC-C1C	3.04	1.44	1.35
14	L5	205	CLA	OBD-CAD	3.04	1.26	1.22
14	J6	1102	CLA	OBD-CAD	3.04	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B2	827	CLA	CHB-C4A	3.04	1.37	1.33
14	A1	821	CLA	OBD-CAD	3.04	1.26	1.22
14	A5	817	CLA	CHB-C4A	3.04	1.37	1.33
14	A5	826	CLA	CHB-C4A	3.04	1.37	1.33
14	B6	825	CLA	OBD-CAD	3.05	1.26	1.22
14	B3	1802	CLA	CHB-C4A	3.05	1.37	1.33
14	A3	802	CLA	CHC-C1C	3.05	1.44	1.35
14	B2	817	CLA	CHC-C1C	3.05	1.44	1.35
14	A4	838	CLA	CHB-C4A	3.05	1.37	1.33
14	L3	204	CLA	OBD-CAD	3.05	1.26	1.22
14	B1	804	CLA	CHC-C1C	3.05	1.44	1.35
14	A6	1608	CLA	CHB-C4A	3.05	1.37	1.33
14	X6	1701	CLA	OBD-CAD	3.05	1.26	1.22
14	A1	807	CLA	OBD-CAD	3.05	1.26	1.22
14	A3	828	CLA	CHC-C1C	3.05	1.44	1.35
14	B6	802	CLA	CHC-C1C	3.05	1.44	1.35
14	A2	1628	CLA	CHC-C1C	3.05	1.44	1.35
14	A2	1606	CLA	OBD-CAD	3.05	1.26	1.22
14	B4	817	CLA	CHB-C4A	3.06	1.37	1.33
14	M2	1201	CLA	O2A-CGA	3.06	1.42	1.33
14	L1	207	CLA	CHB-C4A	3.06	1.37	1.33
14	B3	1842	CLA	CHB-C4A	3.06	1.37	1.33
14	B4	806	CLA	O2A-CGA	3.06	1.42	1.33
14	B3	1815	CLA	OBD-CAD	3.06	1.26	1.22
14	A5	822	CLA	OBD-CAD	3.06	1.26	1.22
14	A3	803	CLA	CHB-C4A	3.06	1.37	1.33
14	B6	805	CLA	OBD-CAD	3.06	1.26	1.22
14	L5	206	CLA	CHB-C4A	3.06	1.37	1.33
14	B5	1821	CLA	OBD-CAD	3.06	1.26	1.22
14	A1	813	CLA	O2D-CGD	3.06	1.40	1.33
14	B2	837	CLA	OBD-CAD	3.06	1.26	1.22
14	B5	1827	CLA	OBD-CAD	3.06	1.26	1.22
14	A4	805	CLA	O2D-CGD	3.06	1.40	1.33
14	X2	1701	CLA	OBD-CAD	3.06	1.26	1.22
14	B4	808	CLA	CHC-C1C	3.06	1.44	1.35
14	B4	830	CLA	CHC-C1C	3.06	1.44	1.35
14	B1	805	CLA	CHB-C4A	3.07	1.37	1.33
16	A2	1650	BCR	C30-C25	3.07	1.58	1.53
14	B2	803	CLA	OBD-CAD	3.07	1.26	1.22
14	A2	1624	CLA	OBD-CAD	3.07	1.26	1.22
14	B1	841	CLA	CHC-C1C	3.07	1.44	1.35
14	A1	805	CLA	O2D-CGD	3.07	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	804	CLA	OBD-CAD	3.07	1.26	1.22
14	A2	1608	CLA	OBD-CAD	3.07	1.26	1.22
14	B3	1803	CLA	CHC-C1C	3.07	1.44	1.35
14	B4	803	CLA	CHC-C1C	3.07	1.44	1.35
14	A6	1626	CLA	CHC-C1C	3.07	1.44	1.35
14	B5	1806	CLA	O2A-CGA	3.07	1.42	1.33
14	B2	805	CLA	CHC-C1C	3.07	1.44	1.35
14	B6	804	CLA	CHC-C1C	3.07	1.44	1.35
14	B2	822	CLA	OBD-CAD	3.07	1.26	1.22
14	B2	828	CLA	CHC-C1C	3.07	1.44	1.35
14	I1	101	CLA	CHB-C4A	3.08	1.37	1.33
14	A3	826	CLA	CHC-C1C	3.08	1.44	1.35
16	L4	208	BCR	C1-C6	3.08	1.58	1.53
14	B6	840	CLA	CHB-C4A	3.08	1.37	1.33
14	B6	834	CLA	OBD-CAD	3.08	1.26	1.22
14	B4	820	CLA	CHC-C1C	3.08	1.44	1.35
14	B6	818	CLA	CHC-C1C	3.08	1.44	1.35
14	A6	1622	CLA	OBD-CAD	3.08	1.26	1.22
14	A2	1610	CLA	OBD-CAD	3.08	1.26	1.22
14	A5	826	CLA	CHC-C1C	3.08	1.44	1.35
14	A2	1603	CLA	CHC-C1C	3.08	1.44	1.35
14	B4	801	CLA	CHC-C1C	3.08	1.44	1.35
14	B3	1819	CLA	OBD-CAD	3.08	1.26	1.22
14	B1	819	CLA	CHC-C1C	3.08	1.44	1.35
16	L6	201	BCR	C1-C6	3.08	1.58	1.53
14	A3	812	CLA	OBD-CAD	3.09	1.26	1.22
14	A6	1609	CLA	OBD-CAD	3.09	1.26	1.22
14	B5	1830	CLA	CHC-C1C	3.09	1.44	1.35
17	B6	849	LHG	P-O3	3.09	1.71	1.59
14	B5	1819	CLA	OBD-CAD	3.09	1.26	1.22
14	A1	822	CLA	CHB-C4A	3.09	1.37	1.33
14	B3	1823	CLA	OBD-CAD	3.09	1.26	1.22
14	L3	205	CLA	CHB-C4A	3.09	1.37	1.33
14	A1	825	CLA	CHC-C1C	3.09	1.44	1.35
14	A4	810	CLA	OBD-CAD	3.09	1.26	1.22
14	B3	1843	CLA	CHC-C1C	3.09	1.44	1.35
14	A1	810	CLA	OBD-CAD	3.09	1.26	1.22
14	A4	825	CLA	CHC-C1C	3.09	1.44	1.35
14	B5	1808	CLA	CHC-C1C	3.09	1.44	1.35
14	A5	840	CLA	OBD-CAD	3.09	1.26	1.22
17	B2	849	LHG	P-O3	3.09	1.71	1.59
14	B1	807	CLA	CHC-C1C	3.09	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B2	818	CLA	OBD-CAD	3.09	1.26	1.22
14	B1	802	CLA	CHB-C4A	3.09	1.37	1.33
14	B5	1836	CLA	OBD-CAD	3.09	1.26	1.22
14	A6	1617	CLA	CHB-C4A	3.10	1.37	1.33
14	X4	102	CLA	OBD-CAD	3.10	1.26	1.22
14	B1	838	CLA	OBD-CAD	3.10	1.26	1.22
14	A4	827	CLA	CHC-C1C	3.10	1.44	1.35
14	A1	803	CLA	OBD-CAD	3.10	1.26	1.22
14	B5	1816	CLA	CHB-C4A	3.10	1.37	1.33
14	A4	808	CLA	OBD-CAD	3.10	1.26	1.22
14	A6	1612	CLA	CHC-C1C	3.10	1.44	1.35
14	B5	1843	CLA	CHC-C1C	3.10	1.44	1.35
14	A1	837	CLA	O2A-CGA	3.10	1.42	1.33
14	F1	1301	CLA	OBD-CAD	3.10	1.26	1.22
14	B6	836	CLA	OBD-CAD	3.10	1.26	1.22
14	B5	1837	CLA	OBD-CAD	3.10	1.26	1.22
14	A2	1617	CLA	OBD-CAD	3.10	1.26	1.22
14	A4	803	CLA	OBD-CAD	3.10	1.26	1.22
14	B1	801	CLA	CHC-C1C	3.10	1.44	1.35
14	J6	1101	CLA	CHB-C4A	3.10	1.37	1.33
14	B4	815	CLA	OBD-CAD	3.10	1.26	1.22
14	B3	1820	CLA	CHC-C1C	3.11	1.44	1.35
14	A3	809	CLA	OBD-CAD	3.11	1.26	1.22
14	B4	805	CLA	OBD-CAD	3.11	1.26	1.22
14	B6	806	CLA	CHC-C1C	3.11	1.44	1.35
14	A2	1641	CLA	CHB-C4A	3.11	1.37	1.33
14	B6	807	CLA	CHC-C1C	3.11	1.44	1.35
14	B3	1808	CLA	CHC-C1C	3.11	1.44	1.35
14	B4	838	CLA	OBD-CAD	3.11	1.26	1.22
14	A1	837	CLA	OBD-CAD	3.11	1.26	1.22
14	J4	101	CLA	OBD-CAD	3.11	1.26	1.22
14	B6	828	CLA	CHC-C1C	3.11	1.44	1.35
14	A1	839	CLA	CHB-C4A	3.11	1.37	1.33
14	A4	802	CLA	CHB-C4A	3.11	1.37	1.33
14	A4	839	CLA	O2A-CGA	3.11	1.42	1.33
14	B3	1831	CLA	CHC-C1C	3.12	1.44	1.35
14	A3	804	CLA	OBD-CAD	3.12	1.26	1.22
14	B5	1823	CLA	OBD-CAD	3.12	1.26	1.22
14	B5	1815	CLA	OBD-CAD	3.12	1.26	1.22
14	B1	814	CLA	OBD-CAD	3.12	1.26	1.22
14	A1	835	CLA	OBD-CAD	3.12	1.26	1.22
14	B6	818	CLA	CHB-C4A	3.12	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B3	1820	CLA	CHB-C4A	3.12	1.37	1.33
14	A1	822	CLA	CHC-C1C	3.12	1.44	1.35
14	B3	1830	CLA	CHC-C1C	3.12	1.44	1.35
14	B2	813	CLA	OBD-CAD	3.12	1.26	1.22
14	A4	834	CLA	OBD-CAD	3.12	1.26	1.22
14	B6	814	CLA	OBD-CAD	3.12	1.26	1.22
14	A2	1605	CLA	CHB-C4A	3.12	1.37	1.33
14	B5	1804	CLA	CHB-C4A	3.12	1.37	1.33
14	A2	1642	CLA	OBD-CAD	3.13	1.26	1.22
14	B1	815	CLA	OBD-CAD	3.13	1.26	1.22
14	B3	1822	CLA	OBD-CAD	3.13	1.26	1.22
14	L2	207	CLA	OBD-CAD	3.13	1.26	1.22
14	A2	1619	CLA	CHB-C4A	3.13	1.37	1.33
16	A6	1646	BCR	C30-C25	3.13	1.58	1.53
14	A1	815	CLA	OBD-CAD	3.13	1.26	1.22
14	J3	101	CLA	OBD-CAD	3.13	1.26	1.22
14	A5	814	CLA	OBD-CAD	3.13	1.26	1.22
14	B4	820	CLA	CHB-C4A	3.13	1.37	1.33
14	B1	829	CLA	CHC-C1C	3.14	1.44	1.35
14	A5	809	CLA	OBD-CAD	3.14	1.26	1.22
14	B6	823	CLA	OBD-CAD	3.14	1.26	1.22
17	A1	848	LHG	P-O3	3.14	1.72	1.59
16	L3	201	BCR	C1-C6	3.14	1.58	1.53
14	L1	206	CLA	OBD-CAD	3.14	1.26	1.22
14	B1	819	CLA	CHB-C4A	3.14	1.37	1.33
14	M6	1201	CLA	O2A-CGA	3.14	1.42	1.33
14	A2	1625	CLA	CHC-C1C	3.14	1.44	1.35
14	B5	1817	CLA	CHB-C4A	3.14	1.37	1.33
14	B2	829	CLA	CHB-C4A	3.14	1.37	1.33
14	A4	841	CLA	CHB-C4A	3.14	1.37	1.33
14	B4	831	CLA	CHC-C1C	3.15	1.44	1.35
14	J5	101	CLA	OBD-CAD	3.15	1.26	1.22
14	B3	1825	CLA	OBD-CAD	3.15	1.26	1.22
14	L5	206	CLA	OBD-CAD	3.15	1.26	1.22
14	B5	1820	CLA	CHB-C4A	3.15	1.37	1.33
14	L3	203	CLA	CHB-C4A	3.15	1.37	1.33
14	B5	1838	CLA	OBD-CAD	3.15	1.26	1.22
14	A4	814	CLA	OBD-CAD	3.15	1.26	1.22
14	B6	829	CLA	CHC-C1C	3.15	1.44	1.35
14	A4	837	CLA	OBD-CAD	3.15	1.26	1.22
14	B5	1810	CLA	OBD-CAD	3.15	1.26	1.22
14	B2	813	CLA	CHB-C4A	3.15	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B4	819	CLA	OBD-CAD	3.15	1.26	1.22
14	A1	814	CLA	OBD-CAD	3.15	1.26	1.22
14	A3	838	CLA	OBD-CAD	3.15	1.26	1.22
14	B2	814	CLA	OBD-CAD	3.15	1.26	1.22
14	J2	101	CLA	OBD-CAD	3.15	1.26	1.22
14	B2	827	CLA	CHC-C1C	3.15	1.44	1.35
14	A5	802	CLA	CHC-C1C	3.15	1.44	1.35
14	B2	837	CLA	CHB-C4A	3.15	1.37	1.33
14	B5	1831	CLA	CHC-C1C	3.15	1.44	1.35
14	A4	815	CLA	OBD-CAD	3.16	1.26	1.22
14	A2	1616	CLA	OBD-CAD	3.16	1.26	1.22
14	A6	1603	CLA	CHC-C1C	3.16	1.44	1.35
14	B4	823	CLA	OBD-CAD	3.16	1.26	1.22
14	A2	1618	CLA	CHB-C4A	3.16	1.37	1.33
14	A4	805	CLA	OBD-CAD	3.16	1.26	1.22
14	B4	837	CLA	OBD-CAD	3.16	1.26	1.22
14	B4	842	CLA	CHB-C4A	3.16	1.37	1.33
14	B5	1816	CLA	OBD-CAD	3.16	1.26	1.22
14	B2	818	CLA	CHB-C4A	3.16	1.37	1.33
14	A6	1611	CLA	OBD-CAD	3.16	1.26	1.22
14	B5	1820	CLA	CHC-C1C	3.16	1.44	1.35
14	B2	833	CLA	OBD-CAD	3.16	1.26	1.22
14	A1	805	CLA	OBD-CAD	3.16	1.26	1.22
14	B6	819	CLA	OBD-CAD	3.16	1.26	1.22
14	J1	101	CLA	OBD-CAD	3.17	1.26	1.22
14	B2	802	CLA	CHB-C4A	3.17	1.37	1.33
14	B2	831	CLA	OBD-CAD	3.17	1.26	1.22
14	A5	808	CLA	CHB-C4A	3.17	1.37	1.33
14	A1	811	CLA	OBD-CAD	3.17	1.26	1.22
14	A2	1601	CLA	OBD-CAD	3.17	1.26	1.22
17	A3	853	LHG	O7-C7	3.17	1.43	1.34
14	B1	830	CLA	CHC-C1C	3.17	1.44	1.35
14	A6	1618	CLA	CHB-C4A	3.17	1.37	1.33
14	B1	837	CLA	OBD-CAD	3.17	1.26	1.22
14	A3	823	CLA	CHC-C1C	3.17	1.44	1.35
14	A3	812	CLA	CHC-C1C	3.17	1.44	1.35
14	B6	825	CLA	CHC-C1C	3.17	1.44	1.35
16	L2	201	BCR	C1-C6	3.18	1.58	1.53
14	A5	823	CLA	CHB-C4A	3.18	1.37	1.33
14	A3	822	CLA	OBD-CAD	3.18	1.26	1.22
14	I6	101	CLA	CHB-C4A	3.18	1.37	1.33
14	B2	824	CLA	CHC-C1C	3.18	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B4	827	CLA	CHC-C1C	3.18	1.44	1.35
14	B1	821	CLA	OBD-CAD	3.18	1.26	1.22
14	B4	832	CLA	CHB-C4A	3.18	1.37	1.33
14	B2	836	CLA	OBD-CAD	3.18	1.26	1.22
14	B4	821	CLA	OBD-CAD	3.18	1.26	1.22
14	A5	812	CLA	CHC-C1C	3.18	1.44	1.35
14	B5	1802	CLA	CHB-C4A	3.18	1.37	1.33
14	B4	836	CLA	OBD-CAD	3.18	1.26	1.22
14	A6	1615	CLA	OBD-CAD	3.18	1.26	1.22
14	A6	1601	CLA	O2D-CGD	3.18	1.41	1.33
14	B6	838	CLA	CHB-C4A	3.18	1.37	1.33
14	A5	842	CLA	CHB-C4A	3.18	1.37	1.33
14	A4	813	CLA	OBD-CAD	3.19	1.26	1.22
14	A4	853	CLA	O2D-CGD	3.19	1.41	1.33
14	A3	816	CLA	CHB-C4A	3.19	1.37	1.33
14	A4	839	CLA	OBD-CAD	3.19	1.26	1.22
14	A4	811	CLA	CHC-C1C	3.19	1.44	1.35
14	A2	1612	CLA	CHB-C4A	3.19	1.37	1.33
14	A1	807	CLA	CHB-C4A	3.19	1.37	1.33
14	A2	1604	CLA	CHC-C1C	3.19	1.44	1.35
14	B1	824	CLA	OBD-CAD	3.19	1.26	1.22
14	A6	1623	CLA	CHB-C4A	3.19	1.37	1.33
14	A2	1614	CLA	CHC-C1C	3.19	1.44	1.35
14	B5	1807	CLA	CHC-C1C	3.19	1.44	1.35
14	B3	1834	CLA	OBD-CAD	3.20	1.26	1.22
14	A5	813	CLA	CHC-C1C	3.20	1.44	1.35
14	A2	1614	CLA	OBD-CAD	3.20	1.26	1.22
14	L6	207	CLA	OBD-CAD	3.20	1.26	1.22
14	A2	1644	CLA	CHB-C4A	3.20	1.37	1.33
14	B3	1821	CLA	CHB-C4A	3.20	1.37	1.33
14	A4	807	CLA	CHB-C4A	3.20	1.37	1.33
16	A1	845	BCR	C30-C25	3.20	1.58	1.53
17	X3	101	LHG	P-O3	3.21	1.72	1.59
14	B1	815	CLA	CHB-C4A	3.21	1.37	1.33
14	B3	1818	CLA	CHB-C4A	3.21	1.37	1.33
14	B1	802	CLA	CHC-C1C	3.21	1.44	1.35
14	A4	836	CLA	OBD-CAD	3.21	1.26	1.22
14	B1	820	CLA	CHB-C4A	3.21	1.37	1.33
14	A1	812	CLA	CHC-C1C	3.21	1.44	1.35
14	B1	810	CLA	CHC-C1C	3.21	1.44	1.35
14	B5	1821	CLA	CHB-C4A	3.21	1.37	1.33
14	B1	833	CLA	OBD-CAD	3.21	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B3	1811	CLA	CHB-C4A	3.21	1.37	1.33
14	K5	102	CLA	OBD-CAD	3.21	1.26	1.22
14	B6	819	CLA	CHB-C4A	3.21	1.37	1.33
14	B4	811	CLA	CHB-C4A	3.21	1.37	1.33
14	B6	838	CLA	OBD-CAD	3.21	1.26	1.22
14	B2	802	CLA	CHC-C1C	3.22	1.44	1.35
14	B5	1832	CLA	CHB-C4A	3.22	1.37	1.33
14	A4	822	CLA	CHB-C4A	3.22	1.37	1.33
14	A3	823	CLA	CHB-C4A	3.22	1.37	1.33
14	A3	813	CLA	CHC-C1C	3.22	1.44	1.35
14	A2	1639	CLA	OBD-CAD	3.22	1.26	1.22
14	B5	1824	CLA	OBD-CAD	3.22	1.26	1.22
14	A4	811	CLA	OBD-CAD	3.22	1.26	1.22
14	A6	1629	CLA	CHC-C1C	3.22	1.44	1.35
17	A6	1649	LHG	O7-C7	3.22	1.43	1.34
14	A2	1618	CLA	OBD-CAD	3.22	1.26	1.22
14	B4	802	CLA	CHC-C1C	3.22	1.44	1.35
14	A5	816	CLA	CHC-C1C	3.22	1.44	1.35
14	B4	810	CLA	CHC-C1C	3.22	1.44	1.35
14	A5	801	CLA	CHC-C1C	3.23	1.44	1.35
14	L3	202	CLA	OBD-CAD	3.23	1.26	1.22
14	B3	1810	CLA	CHC-C1C	3.23	1.44	1.35
14	K6	1401	CLA	OBD-CAD	3.23	1.26	1.22
14	A2	1610	CLA	CHB-C4A	3.23	1.37	1.33
14	A4	822	CLA	CHC-C1C	3.23	1.44	1.35
14	B3	1805	CLA	OBD-CAD	3.23	1.26	1.22
14	K2	1401	CLA	OBD-CAD	3.23	1.26	1.22
14	B3	1827	CLA	CHC-C1C	3.23	1.44	1.35
14	A1	815	CLA	CHC-C1C	3.23	1.44	1.35
14	B6	837	CLA	OBD-CAD	3.23	1.26	1.22
14	A3	839	CLA	OBD-CAD	3.23	1.26	1.22
14	A3	801	CLA	CHC-C1C	3.23	1.44	1.35
14	L2	205	CLA	CHB-C4A	3.23	1.37	1.33
14	B3	1838	CLA	OBD-CAD	3.23	1.26	1.22
14	L3	205	CLA	OBD-CAD	3.23	1.26	1.22
14	A3	829	CLA	CHC-C1C	3.24	1.44	1.35
14	B5	1804	CLA	CHC-C1C	3.24	1.44	1.35
14	A2	1612	CLA	CHC-C1C	3.24	1.44	1.35
14	B3	1804	CLA	CHC-C1C	3.24	1.44	1.35
14	A6	1623	CLA	CHC-C1C	3.24	1.44	1.35
14	A6	1613	CLA	CHC-C1C	3.24	1.44	1.35
14	A3	815	CLA	OBD-CAD	3.24	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A2	1611	CLA	OBD-CAD	3.24	1.26	1.22
14	A2	1601	CLA	O2D-CGD	3.24	1.41	1.33
14	A6	1637	CLA	OBD-CAD	3.24	1.26	1.22
14	A3	816	CLA	CHC-C1C	3.24	1.44	1.35
14	B6	809	CLA	CHB-C4A	3.24	1.37	1.33
14	A5	823	CLA	CHC-C1C	3.24	1.44	1.35
14	A1	808	CLA	OBD-CAD	3.24	1.26	1.22
14	L5	202	CLA	OBD-CAD	3.24	1.26	1.22
14	A6	1610	CLA	CHB-C4A	3.25	1.37	1.33
14	A5	843	CLA	OBD-CAD	3.25	1.27	1.22
14	B5	1811	CLA	CHB-C4A	3.25	1.37	1.33
14	A5	829	CLA	CHC-C1C	3.25	1.44	1.35
14	B5	1827	CLA	CHC-C1C	3.25	1.44	1.35
14	L6	208	CLA	OBD-CAD	3.25	1.27	1.22
14	B4	825	CLA	CHB-C4A	3.25	1.37	1.33
14	B4	804	CLA	CHB-C4A	3.25	1.37	1.33
14	B5	1810	CLA	CHC-C1C	3.25	1.44	1.35
14	B4	821	CLA	CHB-C4A	3.25	1.37	1.33
14	A2	1604	CLA	CHB-C4A	3.25	1.37	1.33
14	A1	811	CLA	CHC-C1C	3.25	1.44	1.35
14	A3	810	CLA	CHC-C1C	3.25	1.44	1.35
14	A6	1601	CLA	OBD-CAD	3.25	1.27	1.22
14	B3	1817	CLA	OBD-CAD	3.25	1.27	1.22
14	B1	806	CLA	OBD-CAD	3.26	1.27	1.22
14	B3	1802	CLA	CHC-C1C	3.26	1.44	1.35
14	A1	801	CLA	CHC-C1C	3.26	1.44	1.35
14	M3	1601	CLA	O2D-CGD	3.26	1.41	1.33
14	A4	812	CLA	CHC-C1C	3.26	1.44	1.35
14	A6	1610	CLA	CHC-C1C	3.26	1.44	1.35
14	B5	1802	CLA	CHC-C1C	3.26	1.44	1.35
14	K3	1401	CLA	OBD-CAD	3.26	1.27	1.22
14	A1	828	CLA	CHC-C1C	3.26	1.44	1.35
14	A2	1602	CLA	CHC-C1C	3.26	1.44	1.35
17	X4	101	LHG	P-O3	3.26	1.72	1.59
14	L3	202	CLA	O2D-CGD	3.26	1.41	1.33
14	A5	810	CLA	CHC-C1C	3.26	1.44	1.35
14	B4	840	CLA	CHB-C4A	3.27	1.37	1.33
14	F2	202	CLA	OBD-CAD	3.27	1.27	1.22
14	A2	1613	CLA	CHC-C1C	3.27	1.44	1.35
14	B4	804	CLA	CHC-C1C	3.27	1.44	1.35
14	A3	808	CLA	CHB-C4A	3.27	1.37	1.33
14	B1	826	CLA	CHC-C1C	3.27	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A6	1609	CLA	CHC-C1C	3.27	1.44	1.35
14	A5	811	CLA	OBD-CAD	3.27	1.27	1.22
16	L5	201	BCR	C1-C6	3.27	1.58	1.53
14	A1	808	CLA	CHC-C1C	3.27	1.44	1.35
14	B3	1810	CLA	OBD-CAD	3.27	1.27	1.22
14	B1	820	CLA	OBD-CAD	3.27	1.27	1.22
14	B4	841	CLA	CHC-C1C	3.27	1.44	1.35
14	A5	819	CLA	OBD-CAD	3.27	1.27	1.22
14	B4	802	CLA	CHB-C4A	3.27	1.37	1.33
14	B5	1840	CLA	CHB-C4A	3.27	1.37	1.33
14	A2	1618	CLA	CHC-C1C	3.27	1.44	1.35
14	B5	1805	CLA	OBD-CAD	3.27	1.27	1.22
14	A5	818	CLA	CHB-C4A	3.27	1.37	1.33
14	L1	207	CLA	OBD-CAD	3.27	1.27	1.22
14	B6	808	CLA	OBD-CAD	3.27	1.27	1.22
14	M3	1601	CLA	OBD-CAD	3.27	1.27	1.22
14	A5	811	CLA	CHC-C1C	3.28	1.44	1.35
14	A3	818	CLA	CHB-C4A	3.28	1.37	1.33
14	A1	809	CLA	CHB-C4A	3.28	1.37	1.33
14	A4	815	CLA	CHC-C1C	3.28	1.44	1.35
14	B4	810	CLA	OBD-CAD	3.28	1.27	1.22
14	B6	830	CLA	CHB-C4A	3.28	1.37	1.33
14	B6	814	CLA	CHB-C4A	3.28	1.37	1.33
14	B3	1840	CLA	CHB-C4A	3.28	1.37	1.33
14	A2	1625	CLA	CHB-C4A	3.28	1.37	1.33
14	A6	1651	CLA	CHC-C1C	3.28	1.44	1.35
14	A4	816	CLA	CHB-C4A	3.28	1.37	1.33
14	B1	805	CLA	CHC-C1C	3.28	1.44	1.35
14	A1	816	CLA	CHB-C4A	3.28	1.37	1.33
14	L5	202	CLA	O2D-CGD	3.28	1.41	1.33
14	B3	1821	CLA	OBD-CAD	3.28	1.27	1.22
14	A2	1615	CLA	CHC-C1C	3.29	1.44	1.35
17	A2	1653	LHG	O7-C7	3.29	1.43	1.34
14	B2	812	CLA	CHC-C1C	3.29	1.44	1.35
17	A4	850	LHG	O7-C7	3.29	1.43	1.34
14	A5	816	CLA	OBD-CAD	3.29	1.27	1.22
14	B1	835	CLA	OBD-CAD	3.29	1.27	1.22
14	B2	835	CLA	OBD-CAD	3.29	1.27	1.22
14	A1	810	CLA	CHC-C1C	3.29	1.44	1.35
14	A5	816	CLA	CHB-C4A	3.29	1.37	1.33
14	A4	815	CLA	CHB-C4A	3.29	1.37	1.33
14	B4	817	CLA	OBD-CAD	3.29	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	810	CLA	CHB-C4A	3.29	1.37	1.33
14	A6	1602	CLA	CHC-C1C	3.29	1.44	1.35
14	F3	202	CLA	OBD-CAD	3.29	1.27	1.22
14	A6	1638	CLA	OBD-CAD	3.29	1.27	1.22
14	K1	1401	CLA	OBD-CAD	3.30	1.27	1.22
14	A6	1640	CLA	CHB-C4A	3.30	1.37	1.33
14	B2	807	CLA	CHC-C1C	3.30	1.44	1.35
14	A1	813	CLA	OBD-CAD	3.30	1.27	1.22
14	A6	1616	CLA	CHC-C1C	3.30	1.44	1.35
14	B5	1834	CLA	OBD-CAD	3.30	1.27	1.22
14	A2	1632	CLA	CHB-C4A	3.30	1.37	1.33
14	B4	852	CLA	OBD-CAD	3.30	1.27	1.22
14	A6	1625	CLA	CHB-C4A	3.30	1.37	1.33
14	A3	811	CLA	CHC-C1C	3.31	1.44	1.35
14	B3	1838	CLA	CHC-C1C	3.31	1.44	1.35
14	B5	1825	CLA	CHB-C4A	3.31	1.37	1.33
14	A4	828	CLA	CHC-C1C	3.31	1.44	1.35
14	A4	809	CLA	CHB-C4A	3.31	1.37	1.33
14	A6	1640	CLA	OBD-CAD	3.31	1.27	1.22
17	A5	851	LHG	O7-C7	3.31	1.43	1.34
14	A4	829	CLA	CHB-C4A	3.31	1.37	1.33
14	A1	809	CLA	CHC-C1C	3.31	1.44	1.35
16	L1	209	BCR	C1-C6	3.31	1.58	1.53
14	A2	1640	CLA	OBD-CAD	3.31	1.27	1.22
14	B6	808	CLA	CHC-C1C	3.31	1.44	1.35
14	B4	838	CLA	CHC-C1C	3.31	1.44	1.35
14	L1	205	CLA	CHB-C4A	3.31	1.37	1.33
14	B5	1815	CLA	CHC-C1C	3.31	1.44	1.35
14	A6	1611	CLA	CHC-C1C	3.32	1.44	1.35
14	B2	817	CLA	OBD-CAD	3.32	1.27	1.22
14	B2	807	CLA	OBD-CAD	3.32	1.27	1.22
14	A1	815	CLA	CHB-C4A	3.32	1.37	1.33
14	A2	1611	CLA	CHC-C1C	3.32	1.44	1.35
14	A4	801	CLA	CHB-C4A	3.32	1.37	1.33
14	B1	824	CLA	CHB-C4A	3.32	1.37	1.33
14	A6	1634	CLA	CHC-C1C	3.32	1.44	1.35
14	B4	816	CLA	CHB-C4A	3.32	1.37	1.33
14	A1	836	CLA	OBD-CAD	3.32	1.27	1.22
16	B2	842	BCR	C30-C25	3.32	1.58	1.53
14	A4	809	CLA	CHC-C1C	3.32	1.44	1.35
14	F6	202	CLA	OBD-CAD	3.32	1.27	1.22
14	B3	1835	CLA	CHC-C1C	3.32	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A4	842	CLA	CHC-C1C	3.33	1.44	1.35
14	A2	1631	CLA	CHC-C1C	3.33	1.44	1.35
14	A3	835	CLA	CHC-C1C	3.33	1.44	1.35
14	A3	810	CLA	CHB-C4A	3.33	1.37	1.33
17	A1	848	LHG	O7-C7	3.33	1.43	1.34
14	A1	840	CLA	CHC-C1C	3.33	1.44	1.35
14	A1	817	CLA	CHB-C4A	3.33	1.37	1.33
14	A2	1606	CLA	CHC-C1C	3.33	1.44	1.35
14	B3	1816	CLA	CHB-C4A	3.33	1.37	1.33
14	L4	203	CLA	CHB-C4A	3.33	1.37	1.33
14	A2	1617	CLA	CHC-C1C	3.33	1.44	1.35
14	B4	808	CLA	CHB-C4A	3.33	1.37	1.33
14	A5	838	CLA	OBD-CAD	3.33	1.27	1.22
14	B4	815	CLA	CHC-C1C	3.33	1.44	1.35
14	A4	810	CLA	CHC-C1C	3.33	1.44	1.35
14	A2	1643	CLA	OBD-CAD	3.33	1.27	1.22
14	A4	833	CLA	CHC-C1C	3.34	1.44	1.35
14	A6	1616	CLA	CHB-C4A	3.34	1.37	1.33
14	B1	811	CLA	CHB-C4A	3.34	1.37	1.33
14	B5	1841	CLA	CHC-C1C	3.34	1.44	1.35
14	B6	816	CLA	CHB-C4A	3.34	1.37	1.33
14	A4	824	CLA	CHB-C4A	3.34	1.37	1.33
14	A4	801	CLA	CHC-C1C	3.34	1.44	1.35
14	A2	1608	CLA	CHC-C1C	3.35	1.44	1.35
14	A6	1641	CLA	CHC-C1C	3.35	1.44	1.35
14	K4	1401	CLA	OBD-CAD	3.35	1.27	1.22
14	B4	809	CLA	CHB-C4A	3.35	1.37	1.33
14	A5	834	CLA	CHC-C1C	3.35	1.44	1.35
14	A5	833	CLA	CHB-C4A	3.35	1.37	1.33
14	A3	844	CLA	CHC-C1C	3.35	1.44	1.35
14	A1	814	CLA	CHC-C1C	3.35	1.44	1.35
14	A1	803	CLA	CHC-C1C	3.35	1.44	1.35
14	B1	837	CLA	CHC-C1C	3.35	1.44	1.35
14	A3	819	CLA	OBD-CAD	3.35	1.27	1.22
14	B5	1803	CLA	CHB-C4A	3.35	1.37	1.33
14	B3	1816	CLA	CHC-C1C	3.35	1.44	1.35
14	A3	830	CLA	CHB-C4A	3.35	1.37	1.33
14	B2	810	CLA	CHC-C1C	3.36	1.44	1.35
14	B5	1806	CLA	CHC-C1C	3.36	1.44	1.35
14	B4	820	CLA	OBD-CAD	3.36	1.27	1.22
14	L4	205	CLA	CHC-C1C	3.36	1.44	1.35
14	A6	1606	CLA	CHC-C1C	3.36	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A6	1604	CLA	CHC-C1C	3.36	1.44	1.35
14	A1	832	CLA	CHC-C1C	3.36	1.44	1.35
14	A5	815	CLA	CHC-C1C	3.36	1.44	1.35
14	B6	833	CLA	CHC-C1C	3.36	1.44	1.35
14	B3	1815	CLA	CHC-C1C	3.36	1.44	1.35
14	B6	814	CLA	CHC-C1C	3.36	1.44	1.35
14	B6	839	CLA	CHC-C1C	3.36	1.44	1.35
14	K5	101	CLA	CHC-C1C	3.36	1.44	1.35
14	A1	838	CLA	CHB-C4A	3.36	1.37	1.33
14	B1	818	CLA	OBD-CAD	3.36	1.27	1.22
14	B6	815	CLA	OBD-CAD	3.36	1.27	1.22
14	M1	1201	CLA	CHC-C1C	3.37	1.44	1.35
14	A2	1626	CLA	CHC-C1C	3.37	1.44	1.35
14	A6	1635	CLA	CHC-C1C	3.37	1.44	1.35
14	A4	808	CLA	CHC-C1C	3.37	1.44	1.35
14	A3	801	CLA	CHB-C4A	3.37	1.37	1.33
14	B5	1838	CLA	CHC-C1C	3.37	1.44	1.35
14	A1	805	CLA	CHC-C1C	3.37	1.44	1.35
14	L4	205	CLA	OBD-CAD	3.37	1.27	1.22
14	B1	816	CLA	OBD-CAD	3.37	1.27	1.22
14	A5	806	CLA	CHC-C1C	3.37	1.44	1.35
14	A5	809	CLA	CHC-C1C	3.37	1.44	1.35
14	A3	836	CLA	CHC-C1C	3.37	1.44	1.35
14	A3	803	CLA	CHC-C1C	3.37	1.44	1.35
14	A3	825	CLA	CHB-C4A	3.37	1.37	1.33
14	L6	206	CLA	CHB-C4A	3.37	1.37	1.33
14	A2	1645	CLA	CHC-C1C	3.37	1.44	1.35
14	B3	1821	CLA	CHC-C1C	3.37	1.44	1.35
14	B4	816	CLA	CHC-C1C	3.37	1.44	1.35
14	B6	836	CLA	CHC-C1C	3.38	1.44	1.35
14	A3	805	CLA	CHC-C1C	3.38	1.44	1.35
16	B2	843	BCR	C1-C6	3.38	1.58	1.53
14	L6	208	CLA	CHC-C1C	3.38	1.44	1.35
14	B4	818	CLA	CHB-C4A	3.38	1.37	1.33
14	A1	833	CLA	CHC-C1C	3.38	1.44	1.35
14	B1	814	CLA	CHC-C1C	3.38	1.44	1.35
14	F5	1301	CLA	OBD-CAD	3.38	1.27	1.22
14	B3	1841	CLA	CHC-C1C	3.38	1.44	1.35
14	A2	1636	CLA	CHC-C1C	3.38	1.44	1.35
14	A3	809	CLA	CHC-C1C	3.38	1.45	1.35
14	A3	833	CLA	CHB-C4A	3.38	1.37	1.33
14	A4	803	CLA	CHC-C1C	3.38	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B6	832	CLA	OBD-CAD	3.38	1.27	1.22
14	B3	1832	CLA	CHB-C4A	3.38	1.37	1.33
17	X4	101	LHG	P-O6	3.38	1.73	1.59
14	B1	839	CLA	CHB-C4A	3.38	1.37	1.33
14	B1	812	CLA	CHC-C1C	3.38	1.45	1.35
14	B2	835	CLA	CHC-C1C	3.38	1.45	1.35
14	B1	840	CLA	CHC-C1C	3.39	1.45	1.35
14	B4	824	CLA	CHC-C1C	3.39	1.45	1.35
14	A3	824	CLA	CHB-C4A	3.39	1.37	1.33
14	A3	804	CLA	CHC-C1C	3.39	1.45	1.35
14	A5	804	CLA	CHC-C1C	3.39	1.45	1.35
16	B5	1845	BCR	C30-C25	3.39	1.58	1.53
14	A2	1602	CLA	CHB-C4A	3.39	1.37	1.33
14	A4	805	CLA	CHC-C1C	3.39	1.45	1.35
14	A1	831	CLA	CHB-C4A	3.39	1.37	1.33
14	A3	845	CLA	OBD-CAD	3.39	1.27	1.22
14	B5	1801	CLA	OBD-CAD	3.39	1.27	1.22
14	A2	1620	CLA	CHB-C4A	3.39	1.37	1.33
14	A6	1615	CLA	CHC-C1C	3.39	1.45	1.35
14	B2	832	CLA	CHC-C1C	3.40	1.45	1.35
14	B3	1808	CLA	CHB-C4A	3.40	1.37	1.33
14	B2	813	CLA	CHC-C1C	3.40	1.45	1.35
14	B6	829	CLA	OBD-CAD	3.40	1.27	1.22
14	M2	1201	CLA	CHC-C1C	3.40	1.45	1.35
14	B1	819	CLA	OBD-CAD	3.40	1.27	1.22
14	B6	813	CLA	CHC-C1C	3.40	1.45	1.35
14	B2	838	CLA	CHC-C1C	3.40	1.45	1.35
14	A5	835	CLA	CHC-C1C	3.40	1.45	1.35
14	B3	1831	CLA	OBD-CAD	3.40	1.27	1.22
14	A1	823	CLA	CHC-C1C	3.40	1.45	1.35
14	B6	816	CLA	CHC-C1C	3.40	1.45	1.35
14	B4	821	CLA	CHC-C1C	3.40	1.45	1.35
14	B5	1817	CLA	OBD-CAD	3.40	1.27	1.22
14	A4	814	CLA	CHC-C1C	3.40	1.45	1.35
14	A3	815	CLA	CHC-C1C	3.40	1.45	1.35
14	A1	802	CLA	CHC-C1C	3.40	1.45	1.35
14	B2	808	CLA	CHB-C4A	3.40	1.37	1.33
14	M6	1201	CLA	CHB-C4A	3.41	1.37	1.33
14	B4	835	CLA	CHC-C1C	3.41	1.45	1.35
14	B2	811	CLA	CHC-C1C	3.41	1.45	1.35
14	L2	207	CLA	CHC-C1C	3.41	1.45	1.35
14	M6	1201	CLA	CHC-C1C	3.41	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	841	CLA	CHB-C4A	3.41	1.37	1.33
14	A4	817	CLA	CHB-C4A	3.41	1.37	1.33
14	A3	842	CLA	OBD-CAD	3.41	1.27	1.22
14	B5	1834	CLA	CHC-C1C	3.41	1.45	1.35
14	B5	1829	CLA	CHC-C1C	3.41	1.45	1.35
14	B1	834	CLA	CHC-C1C	3.41	1.45	1.35
14	B1	817	CLA	CHC-C1C	3.41	1.45	1.35
14	A5	824	CLA	CHC-C1C	3.41	1.45	1.35
14	A3	817	CLA	CHB-C4A	3.42	1.37	1.33
14	J6	1101	CLA	CHC-C1C	3.42	1.45	1.35
14	B4	806	CLA	CHC-C1C	3.42	1.45	1.35
14	B3	1820	CLA	OBD-CAD	3.42	1.27	1.22
14	B5	1816	CLA	CHC-C1C	3.42	1.45	1.35
14	B2	815	CLA	CHB-C4A	3.42	1.37	1.33
14	A6	1619	CLA	OBD-CAD	3.42	1.27	1.22
14	B3	1832	CLA	CHC-C1C	3.42	1.45	1.35
16	B6	844	BCR	C1-C6	3.42	1.58	1.53
14	A3	839	CLA	CHC-C1C	3.42	1.45	1.35
14	B3	1801	CLA	OBD-CAD	3.42	1.27	1.22
14	A2	1605	CLA	CHC-C1C	3.42	1.45	1.35
14	B5	1835	CLA	CHC-C1C	3.42	1.45	1.35
14	B5	1818	CLA	CHC-C1C	3.43	1.45	1.35
14	B3	1813	CLA	CHC-C1C	3.43	1.45	1.35
14	B1	815	CLA	CHC-C1C	3.43	1.45	1.35
14	L5	204	CLA	CHB-C4A	3.43	1.37	1.33
14	B5	1813	CLA	CHC-C1C	3.43	1.45	1.35
14	A4	837	CLA	CHC-C1C	3.43	1.45	1.35
14	A4	834	CLA	CHC-C1C	3.43	1.45	1.35
14	A2	1606	CLA	CHB-C4A	3.43	1.37	1.33
14	B1	853	CLA	OBD-CAD	3.43	1.27	1.22
14	B3	1818	CLA	CHC-C1C	3.43	1.45	1.35
16	B3	1846	BCR	C1-C6	3.43	1.58	1.53
14	B2	831	CLA	CHC-C1C	3.43	1.45	1.35
14	A3	806	CLA	CHC-C1C	3.43	1.45	1.35
14	A3	824	CLA	CHC-C1C	3.43	1.45	1.35
14	A6	1630	CLA	CHB-C4A	3.43	1.37	1.33
14	B6	830	CLA	CHC-C1C	3.43	1.45	1.35
14	A5	822	CLA	CHB-C4A	3.44	1.37	1.33
14	A5	830	CLA	CHB-C4A	3.44	1.37	1.33
14	B4	832	CLA	CHC-C1C	3.44	1.45	1.35
14	B4	813	CLA	CHC-C1C	3.44	1.45	1.35
14	A4	840	CLA	OBD-CAD	3.44	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A3	805	CLA	CHB-C4A	3.44	1.37	1.33
14	B6	819	CLA	CHC-C1C	3.44	1.45	1.35
14	A5	807	CLA	CHC-C1C	3.44	1.45	1.35
14	A6	1638	CLA	CHC-C1C	3.44	1.45	1.35
14	A1	829	CLA	CHB-C4A	3.44	1.37	1.33
14	A6	1622	CLA	CHB-C4A	3.44	1.37	1.33
14	B3	1828	CLA	CHC-C1C	3.44	1.45	1.35
14	B4	818	CLA	CHC-C1C	3.45	1.45	1.35
14	A6	1624	CLA	CHC-C1C	3.45	1.45	1.35
14	A2	1627	CLA	CHB-C4A	3.45	1.37	1.33
16	B5	1846	BCR	C1-C6	3.45	1.58	1.53
14	M3	1601	CLA	CHC-C1C	3.45	1.45	1.35
14	B2	818	CLA	CHC-C1C	3.45	1.45	1.35
14	K3	1401	CLA	CHC-C1C	3.45	1.45	1.35
14	B6	812	CLA	CHC-C1C	3.45	1.45	1.35
14	B1	831	CLA	CHC-C1C	3.45	1.45	1.35
14	B1	809	CLA	CHB-C4A	3.45	1.37	1.33
14	A4	823	CLA	CHC-C1C	3.45	1.45	1.35
14	B6	832	CLA	CHC-C1C	3.45	1.45	1.35
14	B5	1832	CLA	CHC-C1C	3.45	1.45	1.35
14	B4	814	CLA	CHC-C1C	3.45	1.45	1.35
14	B6	823	CLA	CHB-C4A	3.45	1.37	1.33
14	B6	811	CLA	CHC-C1C	3.45	1.45	1.35
14	A5	841	CLA	OBD-CAD	3.45	1.27	1.22
14	B1	828	CLA	CHC-C1C	3.45	1.45	1.35
14	A5	803	CLA	CHC-C1C	3.45	1.45	1.35
14	A2	1637	CLA	CHC-C1C	3.45	1.45	1.35
17	B2	849	LHG	P-O6	3.45	1.73	1.59
17	B6	849	LHG	P-O6	3.45	1.73	1.59
14	A4	832	CLA	CHB-C4A	3.45	1.37	1.33
14	A4	802	CLA	CHC-C1C	3.45	1.45	1.35
14	B1	808	CLA	CHB-C4A	3.46	1.37	1.33
14	B5	1821	CLA	CHC-C1C	3.46	1.45	1.35
16	B6	843	BCR	C30-C25	3.46	1.58	1.53
14	A1	818	CLA	OBD-CAD	3.46	1.27	1.22
14	B3	1803	CLA	CHB-C4A	3.46	1.37	1.33
14	K1	1401	CLA	CHC-C1C	3.46	1.45	1.35
14	B4	834	CLA	CHC-C1C	3.46	1.45	1.35
14	A4	810	CLA	CHB-C4A	3.46	1.37	1.33
14	A3	839	CLA	CHB-C4A	3.46	1.37	1.33
14	B5	1831	CLA	OBD-CAD	3.47	1.27	1.22
14	L5	206	CLA	CHC-C1C	3.47	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B2	821	CLA	CHC-C1C	3.47	1.45	1.35
14	K5	102	CLA	CHC-C1C	3.47	1.45	1.35
14	A2	1640	CLA	CHC-C1C	3.47	1.45	1.35
14	B2	822	CLA	CHB-C4A	3.47	1.37	1.33
14	B3	1819	CLA	CHC-C1C	3.47	1.45	1.35
14	B2	819	CLA	CHC-C1C	3.47	1.45	1.35
14	A6	1602	CLA	CHB-C4A	3.47	1.37	1.33
14	B5	1820	CLA	OBD-CAD	3.47	1.27	1.22
14	A3	811	CLA	CHB-C4A	3.47	1.37	1.33
14	A6	1632	CLA	CHB-C4A	3.47	1.37	1.33
14	L3	205	CLA	CHC-C1C	3.47	1.45	1.35
14	A6	1604	CLA	CHB-C4A	3.48	1.37	1.33
14	B2	815	CLA	CHC-C1C	3.48	1.45	1.35
14	B2	829	CLA	CHC-C1C	3.48	1.45	1.35
14	K5	102	CLA	CHB-C4A	3.48	1.37	1.33
14	B2	828	CLA	OBD-CAD	3.48	1.27	1.22
14	A5	805	CLA	CHB-C4A	3.48	1.37	1.33
14	K2	1401	CLA	CHB-C4A	3.48	1.37	1.33
14	A3	831	CLA	CHC-C1C	3.48	1.45	1.35
14	B3	1814	CLA	CHC-C1C	3.48	1.45	1.35
14	A6	1605	CLA	CHC-C1C	3.48	1.45	1.35
14	B3	1806	CLA	CHC-C1C	3.48	1.45	1.35
14	A2	1621	CLA	OBD-CAD	3.48	1.27	1.22
14	B1	831	CLA	CHB-C4A	3.48	1.37	1.33
14	A1	812	CLA	CHB-C4A	3.48	1.37	1.33
14	A5	805	CLA	CHC-C1C	3.48	1.45	1.35
14	B5	1819	CLA	CHC-C1C	3.48	1.45	1.35
14	A1	804	CLA	CHC-C1C	3.48	1.45	1.35
14	K2	1401	CLA	CHC-C1C	3.48	1.45	1.35
14	A3	807	CLA	CHC-C1C	3.48	1.45	1.35
14	K4	1401	CLA	CHC-C1C	3.49	1.45	1.35
14	B5	1818	CLA	CHB-C4A	3.49	1.37	1.33
14	A3	842	CLA	CHB-C4A	3.49	1.37	1.33
14	A4	836	CLA	CHC-C1C	3.49	1.45	1.35
14	A2	1624	CLA	CHB-C4A	3.49	1.37	1.33
14	B4	803	CLA	CHB-C4A	3.49	1.37	1.33
14	K6	1401	CLA	CHC-C1C	3.49	1.45	1.35
14	A5	801	CLA	CHB-C4A	3.49	1.37	1.33
14	B3	1833	CLA	CHC-C1C	3.49	1.45	1.35
14	B1	820	CLA	CHC-C1C	3.49	1.45	1.35
14	B5	1809	CLA	CHB-C4A	3.49	1.37	1.33
14	A1	838	CLA	CHC-C1C	3.49	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	X5	102	LHG	P-O6	3.50	1.73	1.59
14	B3	1834	CLA	CHC-C1C	3.50	1.45	1.35
14	A6	1637	CLA	CHC-C1C	3.50	1.45	1.35
14	A3	804	CLA	CHB-C4A	3.50	1.37	1.33
14	B6	817	CLA	CHC-C1C	3.50	1.45	1.35
17	B1	851	LHG	P-O6	3.50	1.73	1.59
17	X3	101	LHG	P-O6	3.50	1.73	1.59
14	K6	1401	CLA	CHB-C4A	3.50	1.37	1.33
14	A1	801	CLA	CHB-C4A	3.50	1.37	1.33
14	B3	1809	CLA	CHB-C4A	3.50	1.37	1.33
14	A1	824	CLA	CHB-C4A	3.50	1.37	1.33
17	A3	853	LHG	O8-C23	3.50	1.43	1.33
14	A4	804	CLA	CHC-C1C	3.50	1.45	1.35
14	B6	804	CLA	CHB-C4A	3.50	1.37	1.33
14	A4	806	CLA	CHC-C1C	3.50	1.45	1.35
14	A2	1639	CLA	CHC-C1C	3.51	1.45	1.35
16	B4	846	BCR	C1-C6	3.51	1.58	1.53
14	B6	818	CLA	OBD-CAD	3.51	1.27	1.22
14	B5	1814	CLA	CHC-C1C	3.51	1.45	1.35
14	A5	838	CLA	CHB-C4A	3.51	1.37	1.33
14	B1	818	CLA	CHC-C1C	3.51	1.45	1.35
14	B4	819	CLA	CHC-C1C	3.51	1.45	1.35
14	A5	804	CLA	CHB-C4A	3.51	1.37	1.33
14	A4	816	CLA	CHC-C1C	3.51	1.45	1.35
14	A5	813	CLA	CHB-C4A	3.51	1.37	1.33
14	A1	816	CLA	CHC-C1C	3.51	1.45	1.35
14	A2	1607	CLA	CHC-C1C	3.51	1.45	1.35
14	B4	806	CLA	CHB-C4A	3.51	1.37	1.33
14	A5	825	CLA	CHB-C4A	3.51	1.37	1.33
14	A1	823	CLA	CHB-C4A	3.52	1.37	1.33
14	A6	1640	CLA	CHC-C1C	3.52	1.45	1.35
14	A1	810	CLA	CHB-C4A	3.52	1.37	1.33
14	B6	825	CLA	CHB-C4A	3.52	1.37	1.33
14	B2	805	CLA	CHB-C4A	3.52	1.37	1.33
14	A3	821	CLA	CHC-C1C	3.52	1.45	1.35
16	B1	844	BCR	C1-C6	3.52	1.58	1.53
14	L3	202	CLA	CHC-C1C	3.52	1.45	1.35
14	A4	820	CLA	CHC-C1C	3.52	1.45	1.35
14	F4	202	CLA	OBD-CAD	3.52	1.27	1.22
14	L1	207	CLA	CHC-C1C	3.52	1.45	1.35
14	A5	838	CLA	CHC-C1C	3.52	1.45	1.35
14	A6	1618	CLA	CHC-C1C	3.52	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B1	813	CLA	CHC-C1C	3.52	1.45	1.35
14	B4	828	CLA	CHC-C1C	3.53	1.45	1.35
14	A4	803	CLA	CHB-C4A	3.53	1.37	1.33
14	A6	1638	CLA	CHB-C4A	3.53	1.37	1.33
14	A4	840	CLA	CHB-C4A	3.53	1.37	1.33
14	K3	1401	CLA	CHB-C4A	3.53	1.37	1.33
14	A2	1643	CLA	CHC-C1C	3.53	1.45	1.35
14	B4	822	CLA	CHC-C1C	3.53	1.45	1.35
14	B4	831	CLA	OBD-CAD	3.53	1.27	1.22
14	A3	817	CLA	CHC-C1C	3.53	1.45	1.35
14	B4	834	CLA	OBD-CAD	3.53	1.27	1.22
14	A2	1643	CLA	CHB-C4A	3.54	1.37	1.33
14	A2	1609	CLA	CHC-C1C	3.54	1.45	1.35
14	A6	1617	CLA	CHC-C1C	3.54	1.45	1.35
16	B1	843	BCR	C30-C25	3.54	1.58	1.53
14	L5	202	CLA	CHC-C1C	3.54	1.45	1.35
14	A6	1609	CLA	CHB-C4A	3.54	1.37	1.33
16	B4	845	BCR	C30-C25	3.54	1.58	1.53
14	B3	1824	CLA	CHC-C1C	3.54	1.45	1.35
14	A6	1606	CLA	CHB-C4A	3.54	1.37	1.33
14	A2	1611	CLA	CHB-C4A	3.54	1.37	1.33
14	A2	1608	CLA	CHB-C4A	3.54	1.37	1.33
14	K4	1401	CLA	CHB-C4A	3.54	1.37	1.33
14	K1	1401	CLA	CHB-C4A	3.54	1.37	1.33
14	B6	807	CLA	CHB-C4A	3.54	1.37	1.33
14	B3	1837	CLA	CHC-C1C	3.55	1.45	1.35
17	A3	854	LHG	O8-C23	3.55	1.43	1.33
14	A1	838	CLA	OBD-CAD	3.55	1.27	1.22
14	B2	824	CLA	CHB-C4A	3.55	1.37	1.33
14	A2	1635	CLA	CHB-C4A	3.55	1.37	1.33
14	B1	833	CLA	CHC-C1C	3.55	1.45	1.35
14	A1	806	CLA	CHC-C1C	3.55	1.45	1.35
14	B2	830	CLA	CHC-C1C	3.55	1.45	1.35
14	A6	1607	CLA	CHC-C1C	3.55	1.45	1.35
14	A2	1619	CLA	CHC-C1C	3.55	1.45	1.35
14	A3	818	CLA	CHC-C1C	3.55	1.45	1.35
14	J5	102	CLA	CHC-C1C	3.55	1.45	1.35
14	A5	841	CLA	CHC-C1C	3.55	1.45	1.35
14	B5	1808	CLA	CHB-C4A	3.55	1.37	1.33
14	B2	801	CLA	CHB-C4A	3.56	1.37	1.33
14	B2	826	CLA	OBD-CAD	3.56	1.27	1.22
14	F6	202	CLA	CHC-C1C	3.56	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A6	1621	CLA	CHC-C1C	3.56	1.45	1.35
14	B1	817	CLA	CHB-C4A	3.56	1.37	1.33
14	A5	817	CLA	CHC-C1C	3.56	1.45	1.35
14	B3	1825	CLA	CHB-C4A	3.56	1.37	1.33
14	A2	1615	CLA	CHB-C4A	3.56	1.37	1.33
14	B2	825	CLA	CHC-C1C	3.56	1.45	1.35
16	B3	1845	BCR	C30-C25	3.56	1.58	1.53
14	B1	832	CLA	CHC-C1C	3.57	1.45	1.35
14	A5	824	CLA	CHB-C4A	3.57	1.37	1.33
14	B2	816	CLA	CHC-C1C	3.57	1.45	1.35
17	A4	850	LHG	O8-C23	3.57	1.43	1.33
14	B3	1829	CLA	CHC-C1C	3.57	1.45	1.35
14	A3	838	CLA	CHC-C1C	3.57	1.45	1.35
14	B1	821	CLA	CHC-C1C	3.57	1.45	1.35
14	A1	804	CLA	CHB-C4A	3.57	1.37	1.33
14	B1	830	CLA	OBD-CAD	3.58	1.27	1.22
14	B3	1817	CLA	CHC-C1C	3.58	1.45	1.35
14	B6	831	CLA	CHC-C1C	3.58	1.45	1.35
14	A5	837	CLA	CHC-C1C	3.58	1.45	1.35
14	A1	836	CLA	CHC-C1C	3.58	1.45	1.35
14	A4	817	CLA	CHC-C1C	3.58	1.45	1.35
14	A2	1623	CLA	CHC-C1C	3.58	1.45	1.35
14	B6	826	CLA	CHC-C1C	3.58	1.45	1.35
14	A4	818	CLA	OBD-CAD	3.59	1.27	1.22
14	B5	1833	CLA	CHC-C1C	3.59	1.45	1.35
14	F2	202	CLA	CHC-C1C	3.59	1.45	1.35
14	B6	822	CLA	CHC-C1C	3.59	1.45	1.35
14	J3	102	CLA	CHC-C1C	3.59	1.45	1.35
14	B5	1824	CLA	CHC-C1C	3.59	1.45	1.35
14	A6	1624	CLA	CHB-C4A	3.59	1.37	1.33
14	B1	823	CLA	CHC-C1C	3.59	1.45	1.35
14	A2	1601	CLA	CHC-C1C	3.60	1.45	1.35
14	B5	1828	CLA	CHC-C1C	3.60	1.45	1.35
14	F5	1301	CLA	CHC-C1C	3.60	1.45	1.35
14	J1	102	CLA	CHC-C1C	3.60	1.45	1.35
14	B6	827	CLA	CHC-C1C	3.60	1.45	1.35
14	F1	1301	CLA	CHC-C1C	3.60	1.45	1.35
14	B2	814	CLA	CHC-C1C	3.60	1.45	1.35
14	B2	826	CLA	CHC-C1C	3.60	1.45	1.35
14	A6	1601	CLA	CHC-C1C	3.60	1.45	1.35
14	A2	1633	CLA	CHC-C1C	3.61	1.45	1.35
14	A1	836	CLA	CHB-C4A	3.61	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	831	CLA	CHC-C1C	3.61	1.45	1.35
14	B2	806	CLA	CHB-C4A	3.61	1.37	1.33
17	A5	852	LHG	O8-C23	3.61	1.43	1.33
14	B2	822	CLA	CHC-C1C	3.61	1.45	1.35
14	J6	1103	CLA	CHC-C1C	3.61	1.45	1.35
14	A1	817	CLA	CHC-C1C	3.61	1.45	1.35
14	B4	829	CLA	CHC-C1C	3.62	1.45	1.35
14	A3	842	CLA	CHC-C1C	3.62	1.45	1.35
14	A4	840	CLA	CHC-C1C	3.62	1.45	1.35
14	B4	833	CLA	CHC-C1C	3.62	1.45	1.35
14	F3	202	CLA	CHC-C1C	3.62	1.45	1.35
14	A6	1631	CLA	CHC-C1C	3.62	1.45	1.35
14	B3	1822	CLA	CHC-C1C	3.62	1.45	1.35
14	A2	1613	CLA	CHB-C4A	3.62	1.37	1.33
17	A6	1649	LHG	O8-C23	3.63	1.43	1.33
14	B3	1806	CLA	CHB-C4A	3.63	1.37	1.33
14	A1	821	CLA	CHB-C4A	3.63	1.37	1.33
14	J4	102	CLA	CHC-C1C	3.63	1.45	1.35
14	B5	1806	CLA	CHB-C4A	3.63	1.37	1.33
14	A4	830	CLA	CHC-C1C	3.63	1.45	1.35
14	F2	204	CLA	CHC-C1C	3.63	1.45	1.35
14	B6	820	CLA	CHC-C1C	3.63	1.45	1.35
14	A1	830	CLA	CHC-C1C	3.63	1.45	1.35
14	A4	837	CLA	CHB-C4A	3.64	1.37	1.33
14	B6	815	CLA	CHC-C1C	3.64	1.45	1.35
14	A1	835	CLA	CHC-C1C	3.64	1.45	1.35
14	B5	1817	CLA	CHC-C1C	3.64	1.45	1.35
14	F4	202	CLA	CHC-C1C	3.64	1.45	1.35
14	B1	816	CLA	CHC-C1C	3.64	1.45	1.35
14	A2	1626	CLA	CHB-C4A	3.65	1.37	1.33
14	J6	1102	CLA	CHC-C1C	3.65	1.45	1.35
14	A4	821	CLA	CHB-C4A	3.65	1.37	1.33
14	B1	827	CLA	CHC-C1C	3.65	1.45	1.35
14	B4	817	CLA	CHC-C1C	3.65	1.45	1.35
14	A3	822	CLA	CHB-C4A	3.65	1.37	1.33
14	B6	837	CLA	CHC-C1C	3.65	1.45	1.35
14	B4	827	CLA	CHB-C4A	3.65	1.37	1.33
14	A6	1613	CLA	CHB-C4A	3.65	1.37	1.33
14	A6	1605	CLA	CHB-C4A	3.66	1.37	1.33
14	A3	807	CLA	CHB-C4A	3.66	1.37	1.33
14	A4	853	CLA	CHC-C1C	3.66	1.45	1.35
14	B6	835	CLA	CHC-C1C	3.66	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A4	823	CLA	CHB-C4A	3.66	1.37	1.33
14	B5	1822	CLA	CHC-C1C	3.66	1.45	1.35
14	A4	805	CLA	CHB-C4A	3.66	1.37	1.33
14	A5	821	CLA	CHC-C1C	3.66	1.45	1.35
14	A5	818	CLA	CHC-C1C	3.66	1.45	1.35
14	J4	101	CLA	CHC-C1C	3.66	1.45	1.35
14	A3	809	CLA	CHB-C4A	3.66	1.37	1.33
14	A2	1620	CLA	CHC-C1C	3.66	1.45	1.35
14	B5	1837	CLA	CHC-C1C	3.67	1.45	1.35
14	A3	820	CLA	CHC-C1C	3.67	1.45	1.35
14	J2	101	CLA	CHC-C1C	3.67	1.45	1.35
14	A5	812	CLA	CHB-C4A	3.67	1.37	1.33
14	B3	1836	CLA	CHB-C4A	3.67	1.37	1.33
14	B4	825	CLA	CHC-C1C	3.67	1.45	1.35
14	A5	811	CLA	CHB-C4A	3.67	1.37	1.33
14	A3	806	CLA	CHB-C4A	3.67	1.37	1.33
14	B4	837	CLA	CHC-C1C	3.67	1.45	1.35
17	A2	1653	LHG	O8-C23	3.67	1.44	1.33
14	A5	820	CLA	CHC-C1C	3.68	1.45	1.35
14	A2	1627	CLA	CHC-C1C	3.68	1.45	1.35
14	A1	820	CLA	CHC-C1C	3.68	1.45	1.35
14	A3	814	CLA	CHC-C1C	3.68	1.45	1.35
14	A1	808	CLA	CHB-C4A	3.68	1.37	1.33
14	A3	813	CLA	CHB-C4A	3.68	1.37	1.33
17	A6	1650	LHG	O8-C23	3.68	1.44	1.33
17	A2	1654	LHG	O8-C23	3.68	1.44	1.33
17	A1	848	LHG	O8-C23	3.68	1.44	1.33
14	L2	206	CLA	CHC-C1C	3.69	1.45	1.35
14	B1	828	CLA	OBD-CAD	3.69	1.27	1.22
14	B6	834	CLA	CHC-C1C	3.69	1.45	1.35
14	A4	812	CLA	CHB-C4A	3.69	1.37	1.33
14	J3	101	CLA	CHC-C1C	3.69	1.45	1.35
14	A2	1607	CLA	CHB-C4A	3.70	1.37	1.33
14	A1	803	CLA	CHB-C4A	3.70	1.37	1.33
14	A2	1624	CLA	CHC-C1C	3.70	1.45	1.35
14	A2	1622	CLA	CHC-C1C	3.70	1.45	1.35
14	L3	204	CLA	CHC-C1C	3.70	1.45	1.35
19	B2	848	LMG	O8-C28	3.70	1.44	1.33
14	B1	824	CLA	CHC-C1C	3.70	1.45	1.35
14	B6	823	CLA	CHC-C1C	3.70	1.45	1.35
14	A3	835	CLA	CHB-C4A	3.70	1.37	1.33
14	L1	206	CLA	CHC-C1C	3.70	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B5	1839	CLA	CHC-C1C	3.71	1.45	1.35
14	B2	833	CLA	CHC-C1C	3.71	1.45	1.35
14	B1	841	CLA	CHB-C4A	3.71	1.37	1.33
14	B3	1827	CLA	CHB-C4A	3.71	1.37	1.33
14	B1	838	CLA	CHC-C1C	3.71	1.45	1.35
19	B6	848	LMG	O8-C28	3.71	1.44	1.33
19	B3	1850	LMG	O8-C28	3.71	1.44	1.33
14	B6	834	CLA	CHB-C4A	3.71	1.37	1.33
14	A5	835	CLA	CHB-C4A	3.72	1.37	1.33
14	B6	841	CLA	CHB-C4A	3.72	1.37	1.33
14	A1	801	CLA	OBD-CAD	3.72	1.27	1.22
14	A6	1611	CLA	CHB-C4A	3.72	1.37	1.33
14	B2	821	CLA	CHB-C4A	3.72	1.37	1.33
14	A5	809	CLA	CHB-C4A	3.72	1.37	1.33
14	B1	804	CLA	CHB-C4A	3.72	1.37	1.33
14	B5	1836	CLA	CHC-C1C	3.72	1.45	1.35
14	B2	836	CLA	CHC-C1C	3.73	1.46	1.35
14	B2	803	CLA	CHC-C1C	3.73	1.46	1.35
14	A1	811	CLA	CHB-C4A	3.73	1.37	1.33
17	A1	849	LHG	O8-C23	3.73	1.44	1.33
14	B3	1839	CLA	CHB-C4A	3.73	1.37	1.33
14	B2	834	CLA	CHC-C1C	3.73	1.46	1.35
14	A6	1625	CLA	CHC-C1C	3.73	1.46	1.35
14	L5	205	CLA	CHC-C1C	3.73	1.46	1.35
14	L4	204	CLA	CHC-C1C	3.73	1.46	1.35
14	A4	826	CLA	CHC-C1C	3.73	1.46	1.35
14	A4	804	CLA	CHB-C4A	3.73	1.37	1.33
14	M2	1201	CLA	CHB-C4A	3.73	1.37	1.33
14	A3	845	CLA	CHC-C1C	3.73	1.46	1.35
14	B3	1836	CLA	CHC-C1C	3.73	1.46	1.35
14	B4	829	CLA	OBD-CAD	3.73	1.27	1.22
14	J5	101	CLA	CHC-C1C	3.73	1.46	1.35
14	A3	825	CLA	CHC-C1C	3.73	1.46	1.35
14	L6	207	CLA	CHC-C1C	3.74	1.46	1.35
17	A6	1650	LHG	P-O5	3.74	1.64	1.50
14	B1	836	CLA	CHC-C1C	3.74	1.46	1.35
14	A3	812	CLA	CHB-C4A	3.74	1.37	1.33
17	A5	851	LHG	O8-C23	3.74	1.44	1.33
14	A4	811	CLA	CHB-C4A	3.74	1.37	1.33
14	A6	1622	CLA	CHC-C1C	3.74	1.46	1.35
19	B1	850	LMG	O8-C28	3.74	1.44	1.33
14	A4	838	CLA	CHC-C1C	3.75	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B5	1825	CLA	CHC-C1C	3.75	1.46	1.35
14	X5	101	CLA	CHC-C1C	3.75	1.46	1.35
14	B1	835	CLA	CHB-C4A	3.75	1.37	1.33
14	A3	830	CLA	CHC-C1C	3.75	1.46	1.35
14	B5	1843	CLA	CHB-C4A	3.75	1.37	1.33
14	B3	1839	CLA	CHC-C1C	3.75	1.46	1.35
14	A2	1636	CLA	CHB-C4A	3.75	1.37	1.33
14	A5	814	CLA	CHC-C1C	3.75	1.46	1.35
19	B5	1851	LMG	O8-C28	3.76	1.44	1.33
14	A6	1602	CLA	OBD-CAD	3.76	1.27	1.22
14	A2	1629	CLA	CHC-C1C	3.76	1.46	1.35
14	A6	1627	CLA	CHB-C4A	3.76	1.37	1.33
14	B3	1801	CLA	CHC-C1C	3.76	1.46	1.35
14	B1	826	CLA	CHB-C4A	3.76	1.37	1.33
14	A6	1620	CLA	CHC-C1C	3.76	1.46	1.35
14	X1	1701	CLA	CHC-C1C	3.76	1.46	1.35
14	B4	839	CLA	CHC-C1C	3.76	1.46	1.35
14	A3	822	CLA	CHC-C1C	3.77	1.46	1.35
17	A3	854	LHG	P-O5	3.77	1.64	1.50
14	A6	1612	CLA	CHB-C4A	3.77	1.37	1.33
14	A6	1614	CLA	CHC-C1C	3.77	1.46	1.35
14	J1	101	CLA	CHC-C1C	3.77	1.46	1.35
14	A4	807	CLA	CHC-C1C	3.77	1.46	1.35
14	A5	808	CLA	CHC-C1C	3.77	1.46	1.35
14	A4	819	CLA	CHC-C1C	3.77	1.46	1.35
14	B3	1825	CLA	CHC-C1C	3.77	1.46	1.35
14	A1	824	CLA	CHC-C1C	3.78	1.46	1.35
14	A5	827	CLA	CHC-C1C	3.78	1.46	1.35
14	A3	840	CLA	CHC-C1C	3.78	1.46	1.35
14	X2	1701	CLA	CHC-C1C	3.78	1.46	1.35
14	A1	819	CLA	CHC-C1C	3.78	1.46	1.35
14	A2	1641	CLA	CHC-C1C	3.78	1.46	1.35
14	A5	825	CLA	CHC-C1C	3.78	1.46	1.35
17	A4	851	LHG	O8-C23	3.78	1.44	1.33
14	A6	1608	CLA	CHC-C1C	3.78	1.46	1.35
14	B2	833	CLA	CHB-C4A	3.78	1.37	1.33
14	B1	803	CLA	CHC-C1C	3.79	1.46	1.35
17	A1	849	LHG	P-O5	3.79	1.64	1.50
14	A1	826	CLA	CHC-C1C	3.79	1.46	1.35
14	A1	821	CLA	CHC-C1C	3.79	1.46	1.35
14	A6	1630	CLA	CHC-C1C	3.79	1.46	1.35
14	A5	830	CLA	CHC-C1C	3.79	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A5	839	CLA	CHC-C1C	3.79	1.46	1.35
14	B1	853	CLA	CHC-C1C	3.79	1.46	1.35
14	B2	823	CLA	CHC-C1C	3.79	1.46	1.35
14	B6	822	CLA	CHB-C4A	3.79	1.37	1.33
17	A5	852	LHG	P-O5	3.79	1.64	1.50
14	X3	102	CLA	CHC-C1C	3.79	1.46	1.35
14	A1	813	CLA	CHC-C1C	3.79	1.46	1.35
14	B2	840	CLA	CHB-C4A	3.80	1.37	1.33
14	B4	836	CLA	CHC-C1C	3.80	1.46	1.35
14	F5	1301	CLA	CHB-C4A	3.80	1.37	1.33
14	A2	1637	CLA	CHB-C4A	3.80	1.37	1.33
14	A5	822	CLA	CHC-C1C	3.80	1.46	1.35
14	B6	824	CLA	CHC-C1C	3.80	1.46	1.35
14	B5	1801	CLA	CHC-C1C	3.80	1.46	1.35
14	B3	1823	CLA	CHB-C4A	3.80	1.37	1.33
14	A2	1610	CLA	CHC-C1C	3.80	1.46	1.35
14	L3	203	CLA	CHC-C1C	3.80	1.46	1.35
14	B2	820	CLA	CHC-C1C	3.80	1.46	1.35
14	X4	102	CLA	CHC-C1C	3.80	1.46	1.35
14	F2	202	CLA	CHB-C4A	3.80	1.37	1.33
14	A1	805	CLA	CHB-C4A	3.80	1.37	1.33
14	B5	1823	CLA	CHB-C4A	3.80	1.37	1.33
14	A5	827	CLA	CHB-C4A	3.80	1.37	1.33
14	A4	834	CLA	CHB-C4A	3.81	1.37	1.33
19	B4	851	LMG	O8-C28	3.81	1.44	1.33
14	A2	1632	CLA	CHC-C1C	3.81	1.46	1.35
14	A2	1616	CLA	CHC-C1C	3.81	1.46	1.35
14	B4	852	CLA	CHC-C1C	3.81	1.46	1.35
14	A5	807	CLA	CHB-C4A	3.81	1.37	1.33
14	B4	836	CLA	CHB-C4A	3.81	1.37	1.33
14	B1	835	CLA	CHC-C1C	3.81	1.46	1.35
14	M1	1201	CLA	CHB-C4A	3.81	1.37	1.33
14	A4	821	CLA	CHC-C1C	3.81	1.46	1.35
14	A3	808	CLA	CHC-C1C	3.81	1.46	1.35
14	A6	1607	CLA	CHB-C4A	3.81	1.38	1.33
14	A1	807	CLA	CHC-C1C	3.82	1.46	1.35
14	B5	1836	CLA	CHB-C4A	3.82	1.38	1.33
14	B6	803	CLA	CHC-C1C	3.82	1.46	1.35
17	A4	851	LHG	P-O5	3.82	1.64	1.50
14	A1	829	CLA	CHC-C1C	3.82	1.46	1.35
14	B1	823	CLA	CHB-C4A	3.82	1.38	1.33
14	A6	1627	CLA	CHC-C1C	3.83	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X6	1701	CLA	CHC-C1C	3.83	1.46	1.35
14	A5	801	CLA	OBD-CAD	3.83	1.27	1.22
14	B1	822	CLA	CHC-C1C	3.83	1.46	1.35
14	A2	1614	CLA	CHB-C4A	3.83	1.38	1.33
14	F4	202	CLA	CHB-C4A	3.83	1.38	1.33
14	A3	836	CLA	CHB-C4A	3.83	1.38	1.33
14	A2	1640	CLA	CHB-C4A	3.83	1.38	1.33
14	F3	202	CLA	CHB-C4A	3.83	1.38	1.33
14	A6	1635	CLA	CHB-C4A	3.84	1.38	1.33
14	B1	822	CLA	CHB-C4A	3.84	1.38	1.33
14	A6	1634	CLA	CHB-C4A	3.84	1.38	1.33
14	A4	824	CLA	CHC-C1C	3.84	1.46	1.35
14	B2	820	CLA	CHB-C4A	3.84	1.38	1.33
14	B4	839	CLA	CHB-C4A	3.85	1.38	1.33
14	B5	1823	CLA	CHC-C1C	3.85	1.46	1.35
14	A3	827	CLA	CHC-C1C	3.85	1.46	1.35
14	A3	801	CLA	OBD-CAD	3.85	1.27	1.22
14	L2	205	CLA	CHC-C1C	3.85	1.46	1.35
14	B3	1843	CLA	CHB-C4A	3.85	1.38	1.33
14	A5	843	CLA	CHC-C1C	3.85	1.46	1.35
14	A4	829	CLA	CHC-C1C	3.85	1.46	1.35
14	B2	836	CLA	CHB-C4A	3.85	1.38	1.33
14	B3	1826	CLA	CHC-C1C	3.86	1.46	1.35
14	B6	821	CLA	CHC-C1C	3.86	1.46	1.35
14	L4	203	CLA	CHC-C1C	3.86	1.46	1.35
14	B4	823	CLA	CHB-C4A	3.86	1.38	1.33
14	B6	838	CLA	CHC-C1C	3.86	1.46	1.35
14	A2	1602	CLA	OBD-CAD	3.86	1.27	1.22
14	B3	1824	CLA	CHB-C4A	3.86	1.38	1.33
14	B4	843	CLA	CHB-C4A	3.87	1.38	1.33
14	L6	206	CLA	CHC-C1C	3.87	1.46	1.35
14	A2	1629	CLA	CHB-C4A	3.87	1.38	1.33
17	A2	1654	LHG	P-O5	3.87	1.65	1.50
14	A2	1609	CLA	CHB-C4A	3.87	1.38	1.33
14	L1	205	CLA	CHC-C1C	3.87	1.46	1.35
14	A5	834	CLA	CHB-C4A	3.87	1.38	1.33
14	B1	825	CLA	CHC-C1C	3.87	1.46	1.35
14	B5	1839	CLA	CHB-C4A	3.88	1.38	1.33
14	B4	840	CLA	CHC-C1C	3.88	1.46	1.35
14	L5	204	CLA	CHC-C1C	3.88	1.46	1.35
14	B4	823	CLA	CHC-C1C	3.88	1.46	1.35
14	A4	808	CLA	CHB-C4A	3.89	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B4	826	CLA	CHC-C1C	3.89	1.46	1.35
14	A3	844	CLA	CHB-C4A	3.89	1.38	1.33
14	B5	1827	CLA	CHB-C4A	3.89	1.38	1.33
14	A6	1641	CLA	CHB-C4A	3.89	1.38	1.33
14	B6	837	CLA	CHB-C4A	3.90	1.38	1.33
14	A1	826	CLA	CHB-C4A	3.90	1.38	1.33
14	B5	1826	CLA	CHC-C1C	3.90	1.46	1.35
14	B5	1805	CLA	CHC-C1C	3.90	1.46	1.35
14	A3	820	CLA	CHB-C4A	3.91	1.38	1.33
14	A4	813	CLA	CHC-C1C	3.91	1.46	1.35
14	B3	1823	CLA	CHC-C1C	3.91	1.46	1.35
14	B6	821	CLA	CHB-C4A	3.91	1.38	1.33
14	B6	805	CLA	CHC-C1C	3.91	1.46	1.35
14	A1	832	CLA	CHB-C4A	3.91	1.38	1.33
14	B3	1805	CLA	CHC-C1C	3.92	1.46	1.35
14	F6	202	CLA	CHB-C4A	3.92	1.38	1.33
14	A5	806	CLA	CHB-C4A	3.92	1.38	1.33
14	B1	839	CLA	CHC-C1C	3.93	1.46	1.35
14	B5	1840	CLA	CHC-C1C	3.93	1.46	1.35
14	A1	833	CLA	CHB-C4A	3.93	1.38	1.33
17	X5	102	LHG	O7-C7	3.93	1.45	1.34
14	F1	1301	CLA	CHB-C4A	3.93	1.38	1.33
17	B2	849	LHG	O7-C7	3.95	1.45	1.34
14	B6	827	CLA	OBD-CAD	3.95	1.28	1.22
17	A2	1654	LHG	O7-C7	3.95	1.45	1.34
14	B2	837	CLA	CHC-C1C	3.95	1.46	1.35
14	A3	827	CLA	CHB-C4A	3.95	1.38	1.33
14	B4	805	CLA	CHC-C1C	3.95	1.46	1.35
14	B3	1840	CLA	CHC-C1C	3.95	1.46	1.35
14	B3	1829	CLA	OBD-CAD	3.95	1.28	1.22
14	B1	806	CLA	CHC-C1C	3.96	1.46	1.35
17	A3	853	LHG	P-O5	3.96	1.65	1.50
14	K5	101	CLA	CHB-C4A	3.97	1.38	1.33
17	B6	849	LHG	O7-C7	3.98	1.45	1.34
14	B5	1824	CLA	CHB-C4A	3.98	1.38	1.33
14	A1	819	CLA	CHB-C4A	3.98	1.38	1.33
14	A4	826	CLA	CHB-C4A	3.98	1.38	1.33
17	X4	101	LHG	O7-C7	3.99	1.45	1.34
14	B5	1829	CLA	OBD-CAD	3.99	1.28	1.22
14	B1	807	CLA	CHB-C4A	4.00	1.38	1.33
17	A1	849	LHG	O7-C7	4.00	1.45	1.34
17	A5	852	LHG	O7-C7	4.00	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A4	833	CLA	CHB-C4A	4.01	1.38	1.33
14	A5	820	CLA	CHB-C4A	4.01	1.38	1.33
14	B4	824	CLA	CHB-C4A	4.02	1.38	1.33
14	A4	806	CLA	CHB-C4A	4.02	1.38	1.33
14	B5	1807	CLA	CHB-C4A	4.03	1.38	1.33
17	A4	851	LHG	O7-C7	4.04	1.46	1.34
17	B1	851	LHG	O7-C7	4.04	1.46	1.34
14	A1	840	CLA	CHB-C4A	4.04	1.38	1.33
14	A2	1645	CLA	CHB-C4A	4.05	1.38	1.33
14	A1	806	CLA	CHB-C4A	4.05	1.38	1.33
17	A5	851	LHG	P-O5	4.05	1.65	1.50
14	A6	1620	CLA	CHB-C4A	4.06	1.38	1.33
17	X3	101	LHG	O7-C7	4.06	1.46	1.34
14	B1	838	CLA	CHB-C4A	4.07	1.38	1.33
15	A5	844	PQN	C10-C5	4.08	1.47	1.40
17	A6	1649	LHG	P-O5	4.08	1.65	1.50
17	A3	854	LHG	O7-C7	4.08	1.46	1.34
17	A6	1650	LHG	O7-C7	4.09	1.46	1.34
15	A1	841	PQN	C10-C5	4.09	1.47	1.40
15	A6	1642	PQN	C10-C5	4.09	1.47	1.40
14	B4	807	CLA	CHB-C4A	4.09	1.38	1.33
17	A4	850	LHG	P-O5	4.10	1.65	1.50
15	A3	846	PQN	C10-C5	4.11	1.47	1.40
14	A2	1622	CLA	CHB-C4A	4.11	1.38	1.33
14	A5	829	CLA	CHB-C4A	4.11	1.38	1.33
14	J6	1102	CLA	CHB-C4A	4.12	1.38	1.33
14	B3	1807	CLA	CHB-C4A	4.12	1.38	1.33
14	A3	829	CLA	CHB-C4A	4.13	1.38	1.33
14	A4	842	CLA	CHB-C4A	4.13	1.38	1.33
14	J2	101	CLA	CHB-C4A	4.13	1.38	1.33
14	A4	828	CLA	CHB-C4A	4.14	1.38	1.33
14	B4	831	CLA	CHB-C4A	4.15	1.38	1.33
15	A4	843	PQN	C10-C5	4.15	1.47	1.40
14	B6	829	CLA	CHB-C4A	4.15	1.38	1.33
15	A2	1646	PQN	C10-C5	4.15	1.47	1.40
17	A2	1653	LHG	P-O5	4.15	1.66	1.50
14	J3	101	CLA	CHB-C4A	4.16	1.38	1.33
14	J1	101	CLA	CHB-C4A	4.17	1.38	1.33
14	A6	1629	CLA	CHB-C4A	4.17	1.38	1.33
17	A1	848	LHG	P-O5	4.17	1.66	1.50
14	A4	819	CLA	CHB-C4A	4.19	1.38	1.33
14	J4	101	CLA	CHB-C4A	4.19	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B6	810	CLA	CHB-C4A	4.20	1.38	1.33
14	A4	801	CLA	OBD-CAD	4.21	1.28	1.22
14	B3	1812	CLA	CHB-C4A	4.21	1.38	1.33
14	A2	1631	CLA	CHB-C4A	4.23	1.38	1.33
14	B2	828	CLA	CHB-C4A	4.23	1.38	1.33
14	B4	838	CLA	CHB-C4A	4.23	1.38	1.33
14	J5	101	CLA	CHB-C4A	4.23	1.38	1.33
14	A1	828	CLA	CHB-C4A	4.24	1.38	1.33
15	B2	841	PQN	C10-C5	4.25	1.47	1.40
15	B1	842	PQN	C10-C5	4.25	1.47	1.40
14	B5	1812	CLA	CHB-C4A	4.26	1.38	1.33
14	B2	809	CLA	CHB-C4A	4.26	1.38	1.33
14	B6	806	CLA	CHB-C4A	4.26	1.38	1.33
14	B5	1838	CLA	CHB-C4A	4.28	1.38	1.33
14	B2	804	CLA	CHB-C4A	4.28	1.38	1.33
14	A4	853	CLA	CHB-C4A	4.29	1.38	1.33
15	B4	844	PQN	C10-C5	4.29	1.48	1.40
15	B5	1844	PQN	C10-C5	4.29	1.48	1.40
15	B6	842	PQN	C10-C5	4.32	1.48	1.40
14	B5	1831	CLA	CHB-C4A	4.33	1.38	1.33
17	B1	851	LHG	P-O5	4.34	1.66	1.50
14	M3	1601	CLA	CHB-C4A	4.34	1.38	1.33
17	X3	101	LHG	P-O5	4.34	1.66	1.50
14	B4	812	CLA	CHB-C4A	4.35	1.38	1.33
14	B1	830	CLA	CHB-C4A	4.35	1.38	1.33
15	B3	1844	PQN	C10-C5	4.36	1.48	1.40
14	B5	1822	CLA	CHB-C4A	4.36	1.38	1.33
14	B3	1838	CLA	CHB-C4A	4.37	1.38	1.33
14	B4	822	CLA	CHB-C4A	4.38	1.38	1.33
14	L6	202	CLA	CHB-C4A	4.38	1.38	1.33
17	B2	849	LHG	P-O5	4.39	1.66	1.50
14	A3	832	CLA	CHB-C4A	4.39	1.38	1.33
14	A2	1634	CLA	CHB-C4A	4.41	1.38	1.33
14	B1	837	CLA	CHB-C4A	4.41	1.38	1.33
15	A5	844	PQN	C12-C13	4.41	1.43	1.33
14	B1	821	CLA	CHB-C4A	4.41	1.38	1.33
14	A6	1601	CLA	CHB-C4A	4.42	1.38	1.33
14	J4	102	CLA	CHB-C4A	4.42	1.38	1.33
14	B6	820	CLA	CHB-C4A	4.42	1.38	1.33
15	B5	1844	PQN	C12-C13	4.42	1.43	1.33
15	A3	846	PQN	C12-C13	4.42	1.43	1.33
14	B2	835	CLA	CHB-C4A	4.42	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B1	842	PQN	C12-C13	4.42	1.43	1.33
14	A6	1615	CLA	CHB-C4A	4.43	1.38	1.33
14	B6	836	CLA	CHB-C4A	4.44	1.38	1.33
15	B3	1844	PQN	C12-C13	4.44	1.43	1.33
14	B3	1831	CLA	CHB-C4A	4.44	1.38	1.33
15	A4	843	PQN	C12-C13	4.46	1.44	1.33
14	B2	819	CLA	CHB-C4A	4.46	1.38	1.33
15	B4	844	PQN	C12-C13	4.46	1.44	1.33
14	A6	1639	CLA	CHB-C4A	4.46	1.38	1.33
14	J6	1103	CLA	CHB-C4A	4.47	1.38	1.33
15	A2	1646	PQN	C12-C13	4.47	1.44	1.33
14	J5	102	CLA	CHB-C4A	4.48	1.38	1.33
15	A6	1642	PQN	C12-C13	4.49	1.44	1.33
15	A1	841	PQN	C12-C13	4.49	1.44	1.33
14	A3	815	CLA	CHB-C4A	4.49	1.38	1.33
14	L5	202	CLA	CHB-C4A	4.50	1.38	1.33
15	B2	841	PQN	C12-C13	4.51	1.44	1.33
15	B6	842	PQN	C12-C13	4.51	1.44	1.33
14	L3	202	CLA	CHB-C4A	4.51	1.38	1.33
14	B1	813	CLA	CHB-C4A	4.51	1.38	1.33
14	B3	1822	CLA	CHB-C4A	4.52	1.38	1.33
14	A5	840	CLA	CHB-C4A	4.52	1.38	1.33
14	J1	102	CLA	CHB-C4A	4.53	1.38	1.33
14	F2	204	CLA	CHB-C4A	4.54	1.38	1.33
14	A1	814	CLA	CHB-C4A	4.54	1.38	1.33
14	A5	815	CLA	CHB-C4A	4.57	1.38	1.33
14	A4	831	CLA	CHB-C4A	4.57	1.38	1.33
14	A4	839	CLA	CHB-C4A	4.57	1.38	1.33
14	A4	814	CLA	CHB-C4A	4.58	1.38	1.33
14	A3	841	CLA	CHB-C4A	4.58	1.38	1.33
14	A5	832	CLA	CHB-C4A	4.58	1.38	1.33
14	L1	201	CLA	CHB-C4A	4.58	1.38	1.33
14	A1	837	CLA	CHB-C4A	4.60	1.38	1.33
15	B4	844	PQN	O1-C1	4.62	1.33	1.23
15	B2	841	PQN	O1-C1	4.62	1.33	1.23
15	B3	1844	PQN	O1-C1	4.63	1.33	1.23
14	A2	1617	CLA	CHB-C4A	4.64	1.38	1.33
15	B5	1844	PQN	O1-C1	4.65	1.33	1.23
14	B1	854	CLA	CHB-C4A	4.65	1.38	1.33
15	B1	842	PQN	O1-C1	4.65	1.33	1.23
14	B4	828	CLA	CHB-C4A	4.66	1.38	1.33
15	B6	842	PQN	O1-C1	4.66	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A2	1601	CLA	CHB-C4A	4.67	1.38	1.33
14	B6	812	CLA	CHB-C4A	4.71	1.39	1.33
14	J3	102	CLA	CHB-C4A	4.71	1.39	1.33
14	B6	826	CLA	CHB-C4A	4.75	1.39	1.33
15	B5	1844	PQN	O4-C4	4.76	1.33	1.23
14	X1	1701	CLA	CHB-C4A	4.76	1.39	1.33
14	B5	1828	CLA	CHB-C4A	4.77	1.39	1.33
14	B2	811	CLA	CHB-C4A	4.78	1.39	1.33
15	B4	844	PQN	O4-C4	4.81	1.33	1.23
15	B2	841	PQN	O4-C4	4.82	1.33	1.23
14	B5	1835	CLA	CHB-C4A	4.82	1.39	1.33
14	B5	1814	CLA	CHB-C4A	4.82	1.39	1.33
14	X5	101	CLA	CHB-C4A	4.83	1.39	1.33
14	X3	102	CLA	CHB-C4A	4.84	1.39	1.33
15	B1	842	PQN	O4-C4	4.85	1.33	1.23
15	A1	841	PQN	O1-C1	4.87	1.33	1.23
14	B4	814	CLA	CHB-C4A	4.87	1.39	1.33
15	B6	842	PQN	O4-C4	4.88	1.33	1.23
14	X2	1701	CLA	CHB-C4A	4.89	1.39	1.33
15	A3	846	PQN	O1-C1	4.89	1.33	1.23
15	B3	1844	PQN	O4-C4	4.89	1.33	1.23
14	B3	1828	CLA	CHB-C4A	4.90	1.39	1.33
15	A5	844	PQN	O1-C1	4.92	1.33	1.23
14	B6	833	CLA	CHB-C4A	4.92	1.39	1.33
14	B3	1814	CLA	CHB-C4A	4.92	1.39	1.33
14	A2	1642	CLA	CHB-C4A	4.93	1.39	1.33
15	A6	1642	PQN	O1-C1	4.96	1.33	1.23
15	A1	841	PQN	O4-C4	4.96	1.33	1.23
14	A2	1638	CLA	CHB-C4A	4.97	1.39	1.33
14	A5	836	CLA	CHB-C4A	4.97	1.39	1.33
15	A6	1642	PQN	O4-C4	4.98	1.33	1.23
14	B1	827	CLA	CHB-C4A	4.98	1.39	1.33
14	B2	825	CLA	CHB-C4A	4.99	1.39	1.33
15	A2	1646	PQN	O1-C1	4.99	1.33	1.23
14	B2	832	CLA	CHB-C4A	5.00	1.39	1.33
14	X6	1701	CLA	CHB-C4A	5.00	1.39	1.33
15	A5	844	PQN	O4-C4	5.00	1.33	1.23
15	A3	846	PQN	O4-C4	5.01	1.33	1.23
14	B1	834	CLA	CHB-C4A	5.01	1.39	1.33
15	A2	1646	PQN	O4-C4	5.01	1.33	1.23
15	A4	843	PQN	O1-C1	5.02	1.34	1.23
14	B3	1835	CLA	CHB-C4A	5.03	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A4	843	PQN	O4-C4	5.06	1.34	1.23
14	B4	835	CLA	CHB-C4A	5.10	1.39	1.33
14	A1	834	CLA	CHB-C4A	5.13	1.39	1.33
14	X4	102	CLA	CHB-C4A	5.14	1.39	1.33
14	A6	1636	CLA	CHB-C4A	5.18	1.39	1.33
14	A3	837	CLA	CHB-C4A	5.19	1.39	1.33
14	A4	835	CLA	CHB-C4A	5.24	1.39	1.33
15	B2	841	PQN	C3-C2	5.75	1.47	1.35
15	B1	842	PQN	C3-C2	5.77	1.47	1.35
15	B4	844	PQN	C3-C2	5.79	1.47	1.35
15	B5	1844	PQN	C3-C2	5.81	1.47	1.35
15	B6	842	PQN	C3-C2	5.83	1.47	1.35
15	B3	1844	PQN	C3-C2	5.84	1.47	1.35
15	A6	1642	PQN	C3-C2	5.85	1.47	1.35
15	A1	841	PQN	C3-C2	5.86	1.47	1.35
15	A2	1646	PQN	C3-C2	5.89	1.48	1.35
15	A4	843	PQN	C3-C2	5.95	1.48	1.35
15	A5	844	PQN	C3-C2	5.97	1.48	1.35
15	A3	846	PQN	C3-C2	6.00	1.48	1.35

All (7203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1636	CLA	C1C-NC-C4C	-8.16	102.45	107.05
14	A5	836	CLA	C1C-NC-C4C	-8.14	102.47	107.05
14	A6	1602	CLA	C3D-CAD-CBD	-8.03	96.79	107.61
14	A3	837	CLA	C1C-NC-C4C	-7.98	102.56	107.05
14	A4	801	CLA	C3D-CAD-CBD	-7.88	97.00	107.61
14	A5	801	CLA	C3D-CAD-CBD	-7.86	97.03	107.61
14	A3	801	CLA	C3D-CAD-CBD	-7.81	97.09	107.61
14	A6	1639	CLA	C1C-NC-C4C	-7.79	102.66	107.05
14	B5	1811	CLA	C1C-NC-C4C	-7.78	102.67	107.05
14	A2	1638	CLA	C1C-NC-C4C	-7.78	102.67	107.05
14	A1	834	CLA	C1C-NC-C4C	-7.77	102.67	107.05
14	A3	841	CLA	C1C-NC-C4C	-7.76	102.68	107.05
14	A1	801	CLA	C3D-CAD-CBD	-7.76	97.15	107.61
14	A4	835	CLA	C1C-NC-C4C	-7.76	102.68	107.05
14	A4	839	CLA	C1C-NC-C4C	-7.73	102.70	107.05
14	B4	811	CLA	C1C-NC-C4C	-7.71	102.70	107.05
14	A2	1602	CLA	C3D-CAD-CBD	-7.70	97.24	107.61
14	B3	1812	CLA	C1C-NC-C4C	-7.70	102.71	107.05
14	B1	854	CLA	C1C-NC-C4C	-7.70	102.72	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A5	840	CLA	C1C-NC-C4C	-7.68	102.73	107.05
14	B3	1811	CLA	C1C-NC-C4C	-7.63	102.75	107.05
14	B1	829	CLA	C1C-NC-C4C	-7.61	102.77	107.05
14	A2	1642	CLA	C1C-NC-C4C	-7.60	102.77	107.05
14	B6	810	CLA	C1C-NC-C4C	-7.57	102.79	107.05
14	A1	837	CLA	C1C-NC-C4C	-7.56	102.79	107.05
14	B6	809	CLA	C1C-NC-C4C	-7.54	102.80	107.05
14	B2	809	CLA	C1C-NC-C4C	-7.53	102.81	107.05
14	A3	801	CLA	C1C-NC-C4C	-7.53	102.81	107.05
14	B4	804	CLA	C1C-NC-C4C	-7.52	102.81	107.05
14	B2	808	CLA	C1C-NC-C4C	-7.51	102.82	107.05
14	B4	842	CLA	C1C-NC-C4C	-7.45	102.85	107.05
14	B2	827	CLA	C1C-NC-C4C	-7.45	102.86	107.05
14	B1	811	CLA	C1C-NC-C4C	-7.43	102.86	107.05
14	I1	101	CLA	C1C-NC-C4C	-7.42	102.87	107.05
14	B5	1812	CLA	C1C-NC-C4C	-7.38	102.89	107.05
14	B5	1842	CLA	C1C-NC-C4C	-7.37	102.90	107.05
14	A6	1651	CLA	C1C-NC-C4C	-7.31	102.94	107.05
14	B2	828	CLA	C1C-NC-C4C	-7.27	102.96	107.05
14	B2	839	CLA	C1C-NC-C4C	-7.25	102.97	107.05
14	A6	1602	CLA	C1C-NC-C4C	-7.24	102.97	107.05
14	B4	830	CLA	C1C-NC-C4C	-7.24	102.97	107.05
14	B5	1830	CLA	C1C-NC-C4C	-7.23	102.97	107.05
14	B6	829	CLA	C1C-NC-C4C	-7.23	102.98	107.05
14	B3	1804	CLA	C1C-NC-C4C	-7.19	103.00	107.05
14	B6	828	CLA	C1C-NC-C4C	-7.17	103.01	107.05
14	B3	1842	CLA	C1C-NC-C4C	-7.16	103.02	107.05
14	B2	802	CLA	C1C-NC-C4C	-7.16	103.02	107.05
14	B5	1804	CLA	C1C-NC-C4C	-7.16	103.02	107.05
14	B6	840	CLA	C1C-NC-C4C	-7.15	103.03	107.05
14	A5	807	CLA	C1C-NC-C4C	-7.14	103.03	107.05
14	B1	810	CLA	C1C-NC-C4C	-7.10	103.05	107.05
14	A3	811	CLA	C1C-NC-C4C	-7.10	103.05	107.05
14	A1	801	CLA	C1C-NC-C4C	-7.09	103.05	107.05
14	B4	812	CLA	C1C-NC-C4C	-7.09	103.05	107.05
14	B1	805	CLA	C1C-NC-C4C	-7.09	103.06	107.05
14	B3	1830	CLA	C1C-NC-C4C	-7.07	103.07	107.05
14	A5	842	CLA	C1C-NC-C4C	-7.04	103.09	107.05
14	A4	806	CLA	C1C-NC-C4C	-7.03	103.09	107.05
14	A5	801	CLA	C1C-NC-C4C	-7.03	103.09	107.05
14	B2	826	CLA	C1C-NC-C4C	-7.03	103.09	107.05
14	A2	1609	CLA	C1C-NC-C4C	-7.01	103.10	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A5	811	CLA	C1C-NC-C4C	-7.01	103.10	107.05
14	A4	801	CLA	C1C-NC-C4C	-6.99	103.11	107.05
14	B3	1810	CLA	C1C-NC-C4C	-6.98	103.12	107.05
14	A1	839	CLA	C1C-NC-C4C	-6.98	103.12	107.05
14	L6	208	CLA	C1C-NC-C4C	-6.98	103.12	107.05
14	L4	205	CLA	C1C-NC-C4C	-6.98	103.12	107.05
14	A1	810	CLA	C1C-NC-C4C	-6.96	103.13	107.05
14	B3	1803	CLA	C1C-NC-C4C	-6.95	103.13	107.05
14	B3	1815	CLA	C1C-NC-C4C	-6.92	103.15	107.05
14	B5	1829	CLA	C1C-NC-C4C	-6.91	103.16	107.05
14	A1	809	CLA	C1C-NC-C4C	-6.90	103.16	107.05
14	B1	828	CLA	C1C-NC-C4C	-6.89	103.17	107.05
14	B4	831	CLA	C1C-NC-C4C	-6.87	103.18	107.05
14	A3	816	CLA	C1C-NC-C4C	-6.87	103.18	107.05
14	B2	814	CLA	C1C-NC-C4C	-6.87	103.18	107.05
14	A2	1602	CLA	C1C-NC-C4C	-6.87	103.18	107.05
14	B4	803	CLA	C1C-NC-C4C	-6.86	103.18	107.05
14	A3	843	CLA	C1C-NC-C4C	-6.86	103.19	107.05
14	B4	817	CLA	C1C-NC-C4C	-6.86	103.19	107.05
14	A6	1616	CLA	C1C-NC-C4C	-6.86	103.19	107.05
14	B5	1810	CLA	C1C-NC-C4C	-6.85	103.19	107.05
14	B4	810	CLA	C1C-NC-C4C	-6.84	103.20	107.05
14	A2	1612	CLA	C1C-NC-C4C	-6.84	103.20	107.05
14	B1	801	CLA	C1C-NC-C4C	-6.82	103.21	107.05
14	B5	1821	CLA	C1C-NC-C4C	-6.82	103.21	107.05
14	F3	202	CLA	C1C-NC-C4C	-6.81	103.21	107.05
14	A6	1610	CLA	C1C-NC-C4C	-6.81	103.22	107.05
14	L3	205	CLA	C1C-NC-C4C	-6.80	103.22	107.05
14	A1	806	CLA	C1C-NC-C4C	-6.80	103.22	107.05
14	A5	810	CLA	C1C-NC-C4C	-6.80	103.22	107.05
14	B2	825	CLA	C1C-NC-C4C	-6.80	103.22	107.05
14	A1	816	CLA	C1C-NC-C4C	-6.79	103.22	107.05
14	A3	807	CLA	C1C-NC-C4C	-6.79	103.22	107.05
14	A6	1611	CLA	C1C-NC-C4C	-6.79	103.23	107.05
14	L6	203	CLA	C1C-NC-C4C	-6.79	103.23	107.05
14	B6	808	CLA	C1C-NC-C4C	-6.78	103.23	107.05
14	A5	817	CLA	C1C-NC-C4C	-6.78	103.23	107.05
14	F1	1301	CLA	C1C-NC-C4C	-6.77	103.23	107.05
14	B4	807	CLA	C1C-NC-C4C	-6.77	103.24	107.05
14	A4	841	CLA	C1C-NC-C4C	-6.76	103.24	107.05
14	A6	1617	CLA	C1C-NC-C4C	-6.76	103.24	107.05
14	A6	1607	CLA	C1C-NC-C4C	-6.75	103.25	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	840	CLA	C1C-NC-C4C	-6.74	103.25	107.05
14	B5	1807	CLA	C1C-NC-C4C	-6.73	103.26	107.05
14	A4	810	CLA	C1C-NC-C4C	-6.72	103.27	107.05
14	A4	816	CLA	C1C-NC-C4C	-6.72	103.27	107.05
14	A5	816	CLA	C1C-NC-C4C	-6.71	103.27	107.05
14	B2	807	CLA	C1C-NC-C4C	-6.69	103.28	107.05
14	B4	815	CLA	C1C-NC-C4C	-6.68	103.29	107.05
14	A2	1618	CLA	C1C-NC-C4C	-6.67	103.29	107.05
14	M2	1201	CLA	C1C-NC-C4C	-6.67	103.29	107.05
14	A2	1613	CLA	C1C-NC-C4C	-6.66	103.30	107.05
14	F6	202	CLA	C1C-NC-C4C	-6.66	103.30	107.05
14	B2	812	CLA	C1C-NC-C4C	-6.66	103.30	107.05
14	B6	813	CLA	C1C-NC-C4C	-6.66	103.30	107.05
14	B3	1817	CLA	C1C-NC-C4C	-6.65	103.30	107.05
14	A4	809	CLA	C1C-NC-C4C	-6.65	103.30	107.05
14	B2	804	CLA	C1C-NC-C4C	-6.65	103.30	107.05
14	A3	817	CLA	C1C-NC-C4C	-6.65	103.31	107.05
14	L1	207	CLA	C1C-NC-C4C	-6.64	103.31	107.05
14	A3	826	CLA	C1C-NC-C4C	-6.64	103.31	107.05
14	B5	1803	CLA	C1C-NC-C4C	-6.64	103.31	107.05
14	B6	804	CLA	C1C-NC-C4C	-6.63	103.31	107.05
14	B3	1831	CLA	C1C-NC-C4C	-6.63	103.31	107.05
14	A1	815	CLA	C1C-NC-C4C	-6.62	103.32	107.05
14	L2	207	CLA	C1C-NC-C4C	-6.62	103.32	107.05
14	B6	827	CLA	C1C-NC-C4C	-6.62	103.32	107.05
14	A2	1632	CLA	C1C-NC-C4C	-6.62	103.32	107.05
14	B1	841	CLA	C1C-NC-C4C	-6.62	103.32	107.05
14	A2	1619	CLA	C1C-NC-C4C	-6.62	103.32	107.05
14	B6	815	CLA	C1C-NC-C4C	-6.62	103.32	107.05
14	B6	839	CLA	C1C-NC-C4C	-6.61	103.33	107.05
14	B2	840	CLA	C1C-NC-C4C	-6.61	103.33	107.05
14	A6	1626	CLA	C1C-NC-C4C	-6.60	103.33	107.05
14	B1	814	CLA	C1C-NC-C4C	-6.60	103.33	107.05
14	A5	804	CLA	C1C-NC-C4C	-6.60	103.33	107.05
14	B1	816	CLA	C1C-NC-C4C	-6.60	103.33	107.05
14	B1	804	CLA	C1C-NC-C4C	-6.58	103.34	107.05
14	A4	828	CLA	C1C-NC-C4C	-6.57	103.35	107.05
14	B1	830	CLA	C1C-NC-C4C	-6.56	103.36	107.05
14	B3	1828	CLA	C1C-NC-C4C	-6.55	103.36	107.05
14	A3	802	CLA	C1C-NC-C4C	-6.55	103.36	107.05
14	L5	206	CLA	C1C-NC-C4C	-6.55	103.36	107.05
14	F5	1301	CLA	C1C-NC-C4C	-6.55	103.36	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A5	802	CLA	C1C-NC-C4C	-6.55	103.36	107.05
14	A2	1611	CLA	C1C-NC-C4C	-6.55	103.36	107.05
14	B2	801	CLA	C1C-NC-C4C	-6.55	103.36	107.05
14	A2	1644	CLA	C1C-NC-C4C	-6.54	103.36	107.05
14	B3	1829	CLA	C1C-NC-C4C	-6.54	103.36	107.05
14	A5	829	CLA	C1C-NC-C4C	-6.54	103.36	107.05
14	B4	806	CLA	C1C-NC-C4C	-6.54	103.36	107.05
14	A4	815	CLA	C1C-NC-C4C	-6.54	103.37	107.05
14	F2	202	CLA	C1C-NC-C4C	-6.53	103.37	107.05
14	A5	833	CLA	C1C-NC-C4C	-6.52	103.38	107.05
14	B4	828	CLA	C1C-NC-C4C	-6.52	103.38	107.05
14	B5	1843	CLA	C1C-NC-C4C	-6.52	103.38	107.05
14	A6	1630	CLA	C1C-NC-C4C	-6.52	103.38	107.05
14	B4	829	CLA	C1C-NC-C4C	-6.51	103.38	107.05
14	B2	818	CLA	C1C-NC-C4C	-6.51	103.38	107.05
14	B5	1817	CLA	C1C-NC-C4C	-6.51	103.38	107.05
14	A4	825	CLA	C1C-NC-C4C	-6.51	103.38	107.05
14	K2	1401	CLA	C1C-NC-C4C	-6.50	103.39	107.05
14	A1	831	CLA	C1C-NC-C4C	-6.50	103.39	107.05
14	A1	828	CLA	C1C-NC-C4C	-6.50	103.39	107.05
14	B6	802	CLA	C1C-NC-C4C	-6.50	103.39	107.05
14	B3	1841	CLA	C1C-NC-C4C	-6.50	103.39	107.05
14	A3	833	CLA	C1C-NC-C4C	-6.49	103.39	107.05
14	B6	806	CLA	C1C-NC-C4C	-6.49	103.39	107.05
14	K3	1401	CLA	C1C-NC-C4C	-6.49	103.39	107.05
14	B5	1818	CLA	C1C-NC-C4C	-6.47	103.40	107.05
14	B4	801	CLA	C1C-NC-C4C	-6.47	103.40	107.05
14	A1	808	CLA	C1C-NC-C4C	-6.47	103.40	107.05
14	A3	810	CLA	C1C-NC-C4C	-6.46	103.41	107.05
14	A4	808	CLA	C1C-NC-C4C	-6.46	103.41	107.05
14	A4	831	CLA	C1C-NC-C4C	-6.46	103.41	107.05
14	K5	102	CLA	C1C-NC-C4C	-6.45	103.42	107.05
14	B3	1807	CLA	C1C-NC-C4C	-6.45	103.42	107.05
14	B1	815	CLA	C1C-NC-C4C	-6.44	103.42	107.05
14	B5	1831	CLA	C1C-NC-C4C	-6.44	103.42	107.05
14	B4	841	CLA	C1C-NC-C4C	-6.44	103.42	107.05
14	L5	203	CLA	C1C-NC-C4C	-6.43	103.43	107.05
14	A1	825	CLA	C1C-NC-C4C	-6.43	103.43	107.05
14	B5	1841	CLA	C1C-NC-C4C	-6.43	103.43	107.05
14	A3	830	CLA	C1C-NC-C4C	-6.42	103.43	107.05
14	B6	841	CLA	C1C-NC-C4C	-6.42	103.43	107.05
14	B5	1816	CLA	C1C-NC-C4C	-6.42	103.43	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1815	CLA	C1C-NC-C4C	-6.41	103.44	107.05
14	F4	202	CLA	C1C-NC-C4C	-6.41	103.44	107.05
14	A1	838	CLA	C1C-NC-C4C	-6.41	103.44	107.05
14	L2	205	CLA	C1C-NC-C4C	-6.40	103.44	107.05
14	A1	829	CLA	C1C-NC-C4C	-6.40	103.44	107.05
14	A5	809	CLA	C1C-NC-C4C	-6.40	103.45	107.05
14	A1	803	CLA	C1C-NC-C4C	-6.39	103.45	107.05
14	A2	1634	CLA	C1C-NC-C4C	-6.39	103.45	107.05
14	M1	1201	CLA	C1C-NC-C4C	-6.39	103.45	107.05
14	A6	1632	CLA	C1C-NC-C4C	-6.38	103.45	107.05
14	A2	1631	CLA	C1C-NC-C4C	-6.38	103.46	107.05
14	A4	829	CLA	C1C-NC-C4C	-6.38	103.46	107.05
14	A3	809	CLA	C1C-NC-C4C	-6.38	103.46	107.05
14	L5	204	CLA	C1C-NC-C4C	-6.38	103.46	107.05
14	M6	1201	CLA	C1C-NC-C4C	-6.37	103.46	107.05
14	B1	820	CLA	C1C-NC-C4C	-6.37	103.46	107.05
14	A2	1603	CLA	C1C-NC-C4C	-6.36	103.47	107.05
14	A2	1606	CLA	C1C-NC-C4C	-6.36	103.47	107.05
14	B4	837	CLA	C1C-NC-C4C	-6.36	103.47	107.05
14	K1	1401	CLA	C1C-NC-C4C	-6.35	103.47	107.05
14	B4	821	CLA	C1C-NC-C4C	-6.35	103.47	107.05
14	B3	1818	CLA	C1C-NC-C4C	-6.34	103.48	107.05
14	A3	829	CLA	C1C-NC-C4C	-6.33	103.48	107.05
14	A6	1638	CLA	C1C-NC-C4C	-6.33	103.48	107.05
14	A4	832	CLA	C1C-NC-C4C	-6.33	103.48	107.05
14	A6	1629	CLA	C1C-NC-C4C	-6.33	103.49	107.05
14	L4	201	CLA	C1C-NC-C4C	-6.32	103.49	107.05
14	A5	826	CLA	C1C-NC-C4C	-6.32	103.49	107.05
14	K4	1401	CLA	C1C-NC-C4C	-6.32	103.49	107.05
14	A3	839	CLA	C1C-NC-C4C	-6.32	103.49	107.05
14	A5	841	CLA	C1C-NC-C4C	-6.31	103.49	107.05
14	L6	202	CLA	C1C-NC-C4C	-6.31	103.49	107.05
14	B1	817	CLA	C1C-NC-C4C	-6.31	103.49	107.05
14	A4	827	CLA	C1C-NC-C4C	-6.31	103.49	107.05
14	B3	1813	CLA	C1C-NC-C4C	-6.31	103.50	107.05
14	L1	202	CLA	C1C-NC-C4C	-6.30	103.50	107.05
14	B6	835	CLA	C1C-NC-C4C	-6.30	103.50	107.05
14	A2	1635	CLA	C1C-NC-C4C	-6.30	103.50	107.05
14	L1	201	CLA	C1C-NC-C4C	-6.29	103.51	107.05
14	A4	803	CLA	C1C-NC-C4C	-6.28	103.51	107.05
14	A2	1604	CLA	C1C-NC-C4C	-6.28	103.51	107.05
14	B2	838	CLA	C1C-NC-C4C	-6.28	103.51	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A2	1630	CLA	C1C-NC-C4C	-6.27	103.52	107.05
14	A4	840	CLA	C1C-NC-C4C	-6.27	103.52	107.05
14	B1	827	CLA	C1C-NC-C4C	-6.27	103.52	107.05
14	A3	834	CLA	C1C-NC-C4C	-6.26	103.52	107.05
14	B6	819	CLA	C1C-NC-C4C	-6.25	103.53	107.05
14	A1	805	CLA	C1C-NC-C4C	-6.25	103.53	107.05
14	B2	834	CLA	C1C-NC-C4C	-6.24	103.53	107.05
14	L6	206	CLA	C1C-NC-C4C	-6.23	103.54	107.05
14	B6	826	CLA	C1C-NC-C4C	-6.23	103.54	107.05
14	A6	1609	CLA	C1C-NC-C4C	-6.22	103.55	107.05
14	A6	1604	CLA	C1C-NC-C4C	-6.21	103.55	107.05
14	L4	203	CLA	C1C-NC-C4C	-6.20	103.56	107.05
14	A3	804	CLA	C1C-NC-C4C	-6.20	103.56	107.05
14	B5	1837	CLA	C1C-NC-C4C	-6.20	103.56	107.05
14	A4	822	CLA	C1C-NC-C4C	-6.20	103.56	107.05
14	A5	830	CLA	C1C-NC-C4C	-6.20	103.56	107.05
14	B4	818	CLA	C1C-NC-C4C	-6.19	103.56	107.05
14	B6	814	CLA	C1C-NC-C4C	-6.19	103.56	107.05
14	B4	843	CLA	C1C-NC-C4C	-6.19	103.57	107.05
14	A6	1633	CLA	C1C-NC-C4C	-6.18	103.57	107.05
14	K6	1401	CLA	C1C-NC-C4C	-6.18	103.57	107.05
14	A1	827	CLA	C1C-NC-C4C	-6.18	103.57	107.05
14	A3	823	CLA	C1C-NC-C4C	-6.17	103.57	107.05
14	A3	828	CLA	C1C-NC-C4C	-6.17	103.57	107.05
14	B3	1843	CLA	C1C-NC-C4C	-6.17	103.58	107.05
14	B4	813	CLA	C1C-NC-C4C	-6.17	103.58	107.05
14	A5	823	CLA	C1C-NC-C4C	-6.16	103.58	107.05
14	B1	807	CLA	C1C-NC-C4C	-6.15	103.58	107.05
14	A4	807	CLA	C1C-NC-C4C	-6.15	103.58	107.05
14	B5	1806	CLA	C1C-NC-C4C	-6.15	103.58	107.05
14	A3	842	CLA	C1C-NC-C4C	-6.15	103.59	107.05
14	B3	1821	CLA	C1C-NC-C4C	-6.14	103.59	107.05
14	B6	816	CLA	C1C-NC-C4C	-6.14	103.59	107.05
14	A6	1619	CLA	C1C-NC-C4C	-6.14	103.59	107.05
14	B2	813	CLA	C1C-NC-C4C	-6.13	103.59	107.05
14	A6	1640	CLA	C1C-NC-C4C	-6.13	103.60	107.05
14	A1	812	CLA	C1C-NC-C4C	-6.13	103.60	107.05
14	A1	807	CLA	C1C-NC-C4C	-6.13	103.60	107.05
14	B1	802	CLA	C1C-NC-C4C	-6.12	103.60	107.05
14	A3	832	CLA	C1C-NC-C4C	-6.12	103.61	107.05
14	B3	1802	CLA	C1C-NC-C4C	-6.11	103.61	107.05
14	A2	1625	CLA	C1C-NC-C4C	-6.11	103.61	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	819	CLA	C1C-NC-C4C	-6.10	103.61	107.05
14	B4	808	CLA	C1C-NC-C4C	-6.10	103.61	107.05
14	A1	836	CLA	C1C-NC-C4C	-6.10	103.61	107.05
14	A2	1628	CLA	C1C-NC-C4C	-6.10	103.61	107.05
14	B5	1828	CLA	C1C-NC-C4C	-6.10	103.62	107.05
14	A6	1628	CLA	C1C-NC-C4C	-6.09	103.62	107.05
14	A5	838	CLA	C1C-NC-C4C	-6.09	103.62	107.05
14	A6	1618	CLA	C1C-NC-C4C	-6.09	103.62	107.05
14	B2	805	CLA	C1C-NC-C4C	-6.08	103.62	107.05
14	B2	835	CLA	C1C-NC-C4C	-6.08	103.63	107.05
14	A4	805	CLA	C1C-NC-C4C	-6.08	103.63	107.05
14	B3	1816	CLA	C1C-NC-C4C	-6.07	103.63	107.05
14	B4	838	CLA	C1C-NC-C4C	-6.07	103.63	107.05
14	L2	202	CLA	C1C-NC-C4C	-6.07	103.63	107.05
14	A5	819	CLA	C1C-NC-C4C	-6.06	103.63	107.05
14	B6	811	CLA	C1C-NC-C4C	-6.06	103.64	107.05
14	L1	205	CLA	C1C-NC-C4C	-6.06	103.64	107.05
14	A5	832	CLA	C1C-NC-C4C	-6.05	103.64	107.05
14	A2	1608	CLA	C1C-NC-C4C	-6.04	103.65	107.05
14	A4	837	CLA	C1C-NC-C4C	-6.04	103.65	107.05
14	B3	1808	CLA	C1C-NC-C4C	-6.04	103.65	107.05
14	B6	807	CLA	C1C-NC-C4C	-6.03	103.65	107.05
14	B1	836	CLA	C1C-NC-C4C	-6.03	103.65	107.05
14	B2	810	CLA	C1C-NC-C4C	-6.02	103.66	107.05
14	A6	1603	CLA	C1C-NC-C4C	-6.02	103.66	107.05
14	A2	1643	CLA	C1C-NC-C4C	-6.01	103.66	107.05
14	B5	1808	CLA	C1C-NC-C4C	-6.01	103.66	107.05
14	A5	824	CLA	C1C-NC-C4C	-6.01	103.67	107.05
14	A1	818	CLA	C1C-NC-C4C	-6.00	103.67	107.05
14	A5	818	CLA	C1C-NC-C4C	-6.00	103.67	107.05
14	B4	816	CLA	C1C-NC-C4C	-6.00	103.67	107.05
14	A2	1615	CLA	C1C-NC-C4C	-6.00	103.67	107.05
14	A5	843	CLA	C1C-NC-C4C	-5.99	103.67	107.05
14	A1	822	CLA	C1C-NC-C4C	-5.99	103.67	107.05
14	B1	818	CLA	C1C-NC-C4C	-5.99	103.68	107.05
14	B5	1802	CLA	C1C-NC-C4C	-5.99	103.68	107.05
14	B6	836	CLA	C1C-NC-C4C	-5.98	103.68	107.05
14	B3	1819	CLA	C1C-NC-C4C	-5.98	103.68	107.05
14	A3	838	CLA	C1C-NC-C4C	-5.98	103.68	107.05
14	A5	808	CLA	C1C-NC-C4C	-5.98	103.68	107.05
14	A3	824	CLA	C1C-NC-C4C	-5.98	103.68	107.05
14	B2	815	CLA	C1C-NC-C4C	-5.98	103.68	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1624	CLA	C1C-NC-C4C	-5.96	103.69	107.05
14	A3	813	CLA	C1C-NC-C4C	-5.96	103.69	107.05
14	B3	1837	CLA	C1C-NC-C4C	-5.96	103.69	107.05
14	A6	1606	CLA	C1C-NC-C4C	-5.95	103.70	107.05
14	A5	828	CLA	C1C-NC-C4C	-5.95	103.70	107.05
14	A6	1637	CLA	C1C-NC-C4C	-5.95	103.70	107.05
14	A4	817	CLA	C1C-NC-C4C	-5.95	103.70	107.05
14	A1	817	CLA	C1C-NC-C4C	-5.94	103.71	107.05
14	A6	1623	CLA	C1C-NC-C4C	-5.93	103.71	107.05
14	B4	802	CLA	C1C-NC-C4C	-5.93	103.71	107.05
14	A5	806	CLA	C1C-NC-C4C	-5.93	103.71	107.05
14	B1	812	CLA	C1C-NC-C4C	-5.92	103.72	107.05
14	A6	1608	CLA	C1C-NC-C4C	-5.92	103.72	107.05
14	X5	101	CLA	C1C-NC-C4C	-5.92	103.72	107.05
14	A1	823	CLA	C1C-NC-C4C	-5.92	103.72	107.05
14	B6	833	CLA	C1C-NC-C4C	-5.91	103.72	107.05
14	B1	837	CLA	C1C-NC-C4C	-5.90	103.72	107.05
14	B5	1813	CLA	C1C-NC-C4C	-5.90	103.72	107.05
14	L3	202	CLA	C1C-NC-C4C	-5.89	103.73	107.05
14	B5	1819	CLA	C1C-NC-C4C	-5.88	103.73	107.05
14	A2	1640	CLA	C1C-NC-C4C	-5.88	103.74	107.05
14	B3	1806	CLA	C1C-NC-C4C	-5.87	103.74	107.05
14	A3	818	CLA	C1C-NC-C4C	-5.87	103.75	107.05
14	B3	1825	CLA	C1C-NC-C4C	-5.86	103.75	107.05
14	B5	1838	CLA	C1C-NC-C4C	-5.86	103.75	107.05
14	L3	203	CLA	C1C-NC-C4C	-5.86	103.75	107.05
14	A4	818	CLA	C1C-NC-C4C	-5.86	103.75	107.05
14	A3	806	CLA	C1C-NC-C4C	-5.85	103.76	107.05
14	A6	1613	CLA	C1C-NC-C4C	-5.84	103.76	107.05
14	B1	824	CLA	C1C-NC-C4C	-5.84	103.76	107.05
14	A4	823	CLA	C1C-NC-C4C	-5.84	103.76	107.05
14	A4	842	CLA	C1C-NC-C4C	-5.84	103.76	107.05
14	A2	1621	CLA	C1C-NC-C4C	-5.84	103.76	107.05
15	A2	1646	PQN	C15-C13-C12	-5.83	109.23	121.10
14	B1	853	CLA	C1C-NC-C4C	-5.83	103.77	107.05
14	B3	1801	CLA	C1C-NC-C4C	-5.83	103.77	107.05
14	A3	808	CLA	C1C-NC-C4C	-5.82	103.77	107.05
14	B6	823	CLA	C1C-NC-C4C	-5.82	103.77	107.05
14	A4	812	CLA	C1C-NC-C4C	-5.82	103.77	107.05
14	B3	1838	CLA	C1C-NC-C4C	-5.82	103.77	107.05
14	B1	826	CLA	C1C-NC-C4C	-5.81	103.78	107.05
14	A5	813	CLA	C1C-NC-C4C	-5.80	103.78	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L5	202	CLA	C1C-NC-C4C	-5.80	103.78	107.05
14	A4	801	CLA	O1D-CGD-CBD	-5.79	113.83	124.58
14	A2	1610	CLA	C1C-NC-C4C	-5.79	103.79	107.05
15	A5	844	PQN	C15-C13-C12	-5.79	109.31	121.10
14	A1	835	CLA	C1C-NC-C4C	-5.79	103.79	107.05
14	A3	845	CLA	C1C-NC-C4C	-5.79	103.79	107.05
14	X1	1701	CLA	C1C-NC-C4C	-5.78	103.79	107.05
14	B5	1827	CLA	C1C-NC-C4C	-5.77	103.80	107.05
14	M3	1601	CLA	C1C-NC-C4C	-5.77	103.80	107.05
14	A5	815	CLA	C1C-NC-C4C	-5.76	103.80	107.05
14	A2	1626	CLA	C1C-NC-C4C	-5.76	103.81	107.05
15	A4	843	PQN	C15-C13-C12	-5.75	109.40	121.10
14	A6	1625	CLA	C1C-NC-C4C	-5.75	103.81	107.05
14	A2	1645	CLA	C1C-NC-C4C	-5.74	103.82	107.05
14	B1	808	CLA	C1C-NC-C4C	-5.74	103.82	107.05
14	B2	821	CLA	C1C-NC-C4C	-5.73	103.82	107.05
15	A6	1642	PQN	C15-C13-C12	-5.73	109.44	121.10
14	A2	1627	CLA	C1C-NC-C4C	-5.73	103.82	107.05
14	A3	836	CLA	C1C-NC-C4C	-5.73	103.82	107.05
14	K5	101	CLA	C1C-NC-C4C	-5.73	103.83	107.05
15	A1	841	PQN	C15-C13-C12	-5.71	109.47	121.10
14	A2	1620	CLA	C1C-NC-C4C	-5.71	103.83	107.05
14	X6	1701	CLA	C1C-NC-C4C	-5.71	103.83	107.05
14	A4	834	CLA	C1C-NC-C4C	-5.71	103.83	107.05
14	J4	101	CLA	C1C-NC-C4C	-5.71	103.83	107.05
14	A5	839	CLA	C1C-NC-C4C	-5.71	103.84	107.05
14	B5	1801	CLA	C1C-NC-C4C	-5.71	103.84	107.05
14	A1	832	CLA	C1C-NC-C4C	-5.70	103.84	107.05
14	B4	825	CLA	C1C-NC-C4C	-5.69	103.84	107.05
14	A5	837	CLA	C1C-NC-C4C	-5.69	103.84	107.05
14	X4	102	CLA	C1C-NC-C4C	-5.69	103.84	107.05
14	A3	835	CLA	C1C-NC-C4C	-5.69	103.85	107.05
14	A6	1634	CLA	C1C-NC-C4C	-5.68	103.85	107.05
14	A6	1635	CLA	C1C-NC-C4C	-5.68	103.85	107.05
14	A5	801	CLA	O1D-CGD-CBD	-5.67	114.06	124.58
15	A3	846	PQN	C15-C13-C12	-5.67	109.56	121.10
14	L6	207	CLA	C1C-NC-C4C	-5.67	103.86	107.05
14	B3	1835	CLA	C1C-NC-C4C	-5.66	103.86	107.05
14	B4	819	CLA	C1C-NC-C4C	-5.66	103.86	107.05
14	A3	844	CLA	C1C-NC-C4C	-5.65	103.86	107.05
14	B2	817	CLA	C1C-NC-C4C	-5.65	103.87	107.05
14	B2	832	CLA	C1C-NC-C4C	-5.65	103.87	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A2	1639	CLA	C1C-NC-C4C	-5.65	103.87	107.05
14	B3	1820	CLA	C1C-NC-C4C	-5.65	103.87	107.05
14	B3	1834	CLA	C1C-NC-C4C	-5.64	103.87	107.05
14	B3	1827	CLA	C1C-NC-C4C	-5.64	103.87	107.05
14	B2	822	CLA	C1C-NC-C4C	-5.64	103.87	107.05
14	B4	827	CLA	C1C-NC-C4C	-5.63	103.88	107.05
14	A5	814	CLA	C1C-NC-C4C	-5.63	103.88	107.05
14	J3	102	CLA	C1C-NC-C4C	-5.62	103.88	107.05
14	B3	1824	CLA	C1C-NC-C4C	-5.61	103.89	107.05
14	B6	822	CLA	C1C-NC-C4C	-5.60	103.89	107.05
14	X3	102	CLA	C1C-NC-C4C	-5.60	103.90	107.05
14	A2	1636	CLA	C1C-NC-C4C	-5.59	103.90	107.05
14	A3	825	CLA	C1C-NC-C4C	-5.59	103.90	107.05
14	A6	1601	CLA	C1C-NC-C4C	-5.58	103.91	107.05
14	A1	801	CLA	O1D-CGD-CBD	-5.57	114.24	124.58
14	A2	1602	CLA	O1D-CGD-CBD	-5.57	114.25	124.58
14	X2	1701	CLA	C1C-NC-C4C	-5.57	103.92	107.05
14	A5	835	CLA	C1C-NC-C4C	-5.56	103.92	107.05
15	B5	1844	PQN	C11-C12-C13	-5.56	117.37	126.79
14	A6	1641	CLA	C1C-NC-C4C	-5.56	103.92	107.05
14	A5	825	CLA	C1C-NC-C4C	-5.56	103.92	107.05
14	A3	814	CLA	C1C-NC-C4C	-5.56	103.92	107.05
14	A3	801	CLA	O1D-CGD-CBD	-5.56	114.27	124.58
14	A3	815	CLA	C1C-NC-C4C	-5.55	103.92	107.05
14	A1	824	CLA	C1C-NC-C4C	-5.55	103.92	107.05
14	B4	852	CLA	C1C-NC-C4C	-5.54	103.93	107.05
14	B6	817	CLA	C1C-NC-C4C	-5.54	103.93	107.05
14	J3	101	CLA	C1C-NC-C4C	-5.54	103.93	107.05
14	B6	825	CLA	C1C-NC-C4C	-5.53	103.93	107.05
14	L1	206	CLA	C1C-NC-C4C	-5.53	103.93	107.05
14	A3	812	CLA	C1C-NC-C4C	-5.53	103.94	107.05
14	A6	1615	CLA	C1C-NC-C4C	-5.53	103.94	107.05
14	L2	206	CLA	C1C-NC-C4C	-5.53	103.94	107.05
14	B4	839	CLA	C1C-NC-C4C	-5.52	103.94	107.05
14	A4	802	CLA	C1C-NC-C4C	-5.52	103.94	107.05
14	A5	834	CLA	C1C-NC-C4C	-5.51	103.94	107.05
14	A6	1614	CLA	C1C-NC-C4C	-5.51	103.94	107.05
14	A1	813	CLA	C1C-NC-C4C	-5.51	103.94	107.05
14	B5	1825	CLA	C1C-NC-C4C	-5.51	103.95	107.05
14	A1	840	CLA	C1C-NC-C4C	-5.51	103.95	107.05
14	A4	824	CLA	C1C-NC-C4C	-5.50	103.95	107.05
14	J6	1103	CLA	C1C-NC-C4C	-5.50	103.95	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	834	CLA	C1C-NC-C4C	-5.50	103.95	107.05
14	L4	204	CLA	C1C-NC-C4C	-5.50	103.95	107.05
14	J6	1102	CLA	C1C-NC-C4C	-5.50	103.95	107.05
14	A6	1602	CLA	O1D-CGD-CBD	-5.49	114.39	124.58
14	F2	204	CLA	C1C-NC-C4C	-5.49	103.96	107.05
14	A4	836	CLA	C1C-NC-C4C	-5.49	103.96	107.05
14	J6	1101	CLA	C1C-NC-C4C	-5.48	103.96	107.05
14	B6	818	CLA	C1C-NC-C4C	-5.47	103.97	107.05
14	B6	832	CLA	C1C-NC-C4C	-5.47	103.97	107.05
14	A2	1617	CLA	C1C-NC-C4C	-5.47	103.97	107.05
14	B4	835	CLA	C1C-NC-C4C	-5.46	103.97	107.05
14	J4	102	CLA	C1C-NC-C4C	-5.46	103.97	107.05
14	A2	1614	CLA	C1C-NC-C4C	-5.46	103.97	107.05
14	A3	805	CLA	C1C-NC-C4C	-5.46	103.98	107.05
15	B4	844	PQN	C11-C12-C13	-5.45	117.55	126.79
14	A2	1637	CLA	C1C-NC-C4C	-5.45	103.98	107.05
14	B5	1835	CLA	C1C-NC-C4C	-5.45	103.98	107.05
14	B5	1834	CLA	C1C-NC-C4C	-5.44	103.99	107.05
14	A4	814	CLA	C1C-NC-C4C	-5.43	103.99	107.05
14	A2	1601	CLA	C1C-NC-C4C	-5.43	103.99	107.05
14	B5	1839	CLA	C1C-NC-C4C	-5.43	103.99	107.05
14	J5	101	CLA	C1C-NC-C4C	-5.42	103.99	107.05
15	B3	1844	PQN	C11-C12-C13	-5.42	117.60	126.79
14	A1	814	CLA	C1C-NC-C4C	-5.42	104.00	107.05
14	B6	803	CLA	C1C-NC-C4C	-5.42	104.00	107.05
14	B1	813	CLA	C1C-NC-C4C	-5.42	104.00	107.05
14	B5	1824	CLA	C1C-NC-C4C	-5.42	104.00	107.05
14	A4	853	CLA	C1C-NC-C4C	-5.42	104.00	107.05
14	J1	102	CLA	C1C-NC-C4C	-5.41	104.00	107.05
14	A4	811	CLA	C1C-NC-C4C	-5.41	104.00	107.05
14	B1	803	CLA	C1C-NC-C4C	-5.41	104.00	107.05
14	B2	824	CLA	C1C-NC-C4C	-5.41	104.00	107.05
14	B3	1839	CLA	C1C-NC-C4C	-5.41	104.00	107.05
15	B1	842	PQN	C11-C12-C13	-5.40	117.64	126.79
15	B2	841	PQN	C11-C12-C13	-5.40	117.64	126.79
14	B2	816	CLA	C1C-NC-C4C	-5.40	104.01	107.05
14	B4	834	CLA	C1C-NC-C4C	-5.40	104.01	107.05
15	B6	842	PQN	C11-C12-C13	-5.39	117.67	126.79
14	A6	1612	CLA	C1C-NC-C4C	-5.39	104.02	107.05
14	A2	1616	CLA	C1C-NC-C4C	-5.38	104.02	107.05
14	B4	820	CLA	C1C-NC-C4C	-5.38	104.02	107.05
14	B4	824	CLA	C1C-NC-C4C	-5.38	104.02	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A4	813	CLA	C1C-NC-C4C	-5.37	104.02	107.05
14	B4	833	CLA	C1C-NC-C4C	-5.36	104.03	107.05
14	A2	1605	CLA	C1C-NC-C4C	-5.36	104.03	107.05
14	J2	101	CLA	C1C-NC-C4C	-5.36	104.03	107.05
14	A1	811	CLA	C1C-NC-C4C	-5.35	104.04	107.05
14	A2	1607	CLA	C1C-NC-C4C	-5.33	104.05	107.05
14	B6	837	CLA	C1C-NC-C4C	-5.33	104.05	107.05
14	B5	1820	CLA	C1C-NC-C4C	-5.33	104.05	107.05
14	L3	204	CLA	C1C-NC-C4C	-5.33	104.05	107.05
14	A5	827	CLA	C1C-NC-C4C	-5.32	104.06	107.05
14	A4	838	CLA	C1C-NC-C4C	-5.31	104.06	107.05
14	B2	831	CLA	C1C-NC-C4C	-5.31	104.06	107.05
15	A2	1646	PQN	C11-C12-C13	-5.30	117.81	126.79
14	A2	1641	CLA	C1C-NC-C4C	-5.28	104.08	107.05
14	A4	833	CLA	C1C-NC-C4C	-5.28	104.08	107.05
14	A1	833	CLA	C1C-NC-C4C	-5.27	104.08	107.05
14	A5	821	CLA	C1C-NC-C4C	-5.27	104.08	107.05
14	B1	809	CLA	C1C-NC-C4C	-5.27	104.08	107.05
14	A5	812	CLA	C1C-NC-C4C	-5.27	104.08	107.05
15	A1	841	PQN	C11-C12-C13	-5.26	117.88	126.79
14	A4	826	CLA	C1C-NC-C4C	-5.26	104.09	107.05
14	B3	1832	CLA	C1C-NC-C4C	-5.24	104.10	107.05
14	B1	823	CLA	C1C-NC-C4C	-5.24	104.10	107.05
14	B5	1809	CLA	C1C-NC-C4C	-5.23	104.11	107.05
14	B1	838	CLA	C1C-NC-C4C	-5.23	104.11	107.05
14	A6	1605	CLA	C1C-NC-C4C	-5.22	104.11	107.05
15	A4	843	PQN	C11-C12-C13	-5.22	117.95	126.79
14	B1	819	CLA	C1C-NC-C4C	-5.22	104.11	107.05
14	A3	840	CLA	C1C-NC-C4C	-5.21	104.11	107.05
14	A5	803	CLA	C1C-NC-C4C	-5.20	104.12	107.05
14	A2	1629	CLA	C1C-NC-C4C	-5.20	104.12	107.05
14	B5	1833	CLA	C1C-NC-C4C	-5.20	104.12	107.05
14	A3	803	CLA	C1C-NC-C4C	-5.19	104.13	107.05
15	A5	844	PQN	C11-C12-C13	-5.19	118.00	126.79
14	A1	802	CLA	C1C-NC-C4C	-5.18	104.13	107.05
14	B2	836	CLA	C1C-NC-C4C	-5.18	104.13	107.05
14	J5	102	CLA	C1C-NC-C4C	-5.18	104.13	107.05
14	B3	1809	CLA	C1C-NC-C4C	-5.17	104.14	107.05
14	B2	830	CLA	C1C-NC-C4C	-5.16	104.14	107.05
14	B6	812	CLA	C1C-NC-C4C	-5.16	104.14	107.05
14	B1	832	CLA	C1C-NC-C4C	-5.15	104.15	107.05
14	B6	824	CLA	C1C-NC-C4C	-5.15	104.15	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A4	804	CLA	C1C-NC-C4C	-5.15	104.15	107.05
14	B2	806	CLA	C1C-NC-C4C	-5.14	104.16	107.05
14	A6	1627	CLA	C1C-NC-C4C	-5.14	104.16	107.05
14	L5	205	CLA	C1C-NC-C4C	-5.13	104.16	107.05
14	B1	825	CLA	C1C-NC-C4C	-5.12	104.17	107.05
14	B6	834	CLA	C1C-NC-C4C	-5.11	104.17	107.05
14	B1	833	CLA	C1C-NC-C4C	-5.11	104.17	107.05
15	A3	846	PQN	C11-C12-C13	-5.07	118.21	126.79
14	B5	1814	CLA	C1C-NC-C4C	-5.06	104.20	107.05
14	A1	826	CLA	C1C-NC-C4C	-5.06	104.20	107.05
14	I6	101	CLA	C1C-NC-C4C	-5.06	104.20	107.05
14	B3	1833	CLA	C1C-NC-C4C	-5.05	104.20	107.05
14	A6	1621	CLA	C1C-NC-C4C	-5.05	104.20	107.05
14	A3	827	CLA	C1C-NC-C4C	-5.04	104.21	107.05
14	J1	101	CLA	C1C-NC-C4C	-5.04	104.21	107.05
14	B3	1823	CLA	C1C-NC-C4C	-5.03	104.21	107.05
15	A6	1642	PQN	C11-C12-C13	-5.03	118.27	126.79
14	A5	805	CLA	C1C-NC-C4C	-5.01	104.23	107.05
14	B3	1814	CLA	C1C-NC-C4C	-5.01	104.23	107.05
14	B2	819	CLA	C1C-NC-C4C	-5.00	104.23	107.05
14	B2	823	CLA	C1C-NC-C4C	-5.00	104.24	107.05
14	B2	811	CLA	C1C-NC-C4C	-4.99	104.24	107.05
14	B5	1822	CLA	C1C-NC-C4C	-4.98	104.25	107.05
14	A2	1623	CLA	C1C-NC-C4C	-4.98	104.25	107.05
14	B4	809	CLA	C1C-NC-C4C	-4.98	104.25	107.05
14	B1	821	CLA	C1C-NC-C4C	-4.97	104.25	107.05
14	B5	1805	CLA	C1C-NC-C4C	-4.96	104.25	107.05
14	B3	1826	CLA	C1C-NC-C4C	-4.93	104.27	107.05
14	B1	822	CLA	C1C-NC-C4C	-4.93	104.27	107.05
14	B4	814	CLA	C1C-NC-C4C	-4.92	104.28	107.05
14	B5	1826	CLA	C1C-NC-C4C	-4.92	104.28	107.05
14	B4	826	CLA	C1C-NC-C4C	-4.91	104.28	107.05
14	B2	803	CLA	C1C-NC-C4C	-4.88	104.30	107.05
14	B3	1836	CLA	C1C-NC-C4C	-4.85	104.32	107.05
14	A4	820	CLA	C1C-NC-C4C	-4.85	104.32	107.05
14	B1	835	CLA	C1C-NC-C4C	-4.84	104.32	107.05
14	B2	833	CLA	C1C-NC-C4C	-4.83	104.33	107.05
14	A3	821	CLA	C1C-NC-C4C	-4.81	104.34	107.05
14	B4	840	CLA	C1C-NC-C4C	-4.81	104.34	107.05
14	B1	839	CLA	C1C-NC-C4C	-4.79	104.35	107.05
14	B4	823	CLA	C1C-NC-C4C	-4.79	104.35	107.05
14	B4	836	CLA	C1C-NC-C4C	-4.75	104.38	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	805	CLA	C1C-NC-C4C	-4.73	104.39	107.05
14	B6	821	CLA	C1C-NC-C4C	-4.73	104.39	107.05
14	B5	1823	CLA	C1C-NC-C4C	-4.73	104.39	107.05
14	B3	1805	CLA	C1C-NC-C4C	-4.72	104.39	107.05
14	A1	804	CLA	C1C-NC-C4C	-4.72	104.39	107.05
14	B5	1840	CLA	C1C-NC-C4C	-4.70	104.40	107.05
14	B4	805	CLA	C1C-NC-C4C	-4.70	104.40	107.05
14	A1	820	CLA	C1C-NC-C4C	-4.70	104.40	107.05
14	B6	830	CLA	C1C-NC-C4C	-4.70	104.40	107.05
14	B6	831	CLA	C1C-NC-C4C	-4.69	104.41	107.05
14	A5	822	CLA	C1C-NC-C4C	-4.69	104.41	107.05
14	B3	1840	CLA	C1C-NC-C4C	-4.65	104.43	107.05
14	B2	820	CLA	C1C-NC-C4C	-4.62	104.45	107.05
14	B5	1836	CLA	C1C-NC-C4C	-4.61	104.45	107.05
14	B6	820	CLA	C1C-NC-C4C	-4.60	104.46	107.05
14	B4	822	CLA	C1C-NC-C4C	-4.59	104.47	107.05
14	A2	1624	CLA	C1C-NC-C4C	-4.58	104.47	107.05
14	A4	821	CLA	C1C-NC-C4C	-4.53	104.50	107.05
14	A3	822	CLA	C1C-NC-C4C	-4.50	104.52	107.05
14	B6	838	CLA	C1C-NC-C4C	-4.49	104.52	107.05
14	A2	1633	CLA	C1C-NC-C4C	-4.49	104.52	107.05
14	B3	1822	CLA	C1C-NC-C4C	-4.48	104.53	107.05
14	B1	806	CLA	C1C-NC-C4C	-4.47	104.53	107.05
14	B4	832	CLA	C1C-NC-C4C	-4.46	104.54	107.05
14	B5	1832	CLA	C1C-NC-C4C	-4.46	104.54	107.05
14	B2	837	CLA	C1C-NC-C4C	-4.45	104.54	107.05
14	A1	821	CLA	C1C-NC-C4C	-4.42	104.56	107.05
14	A6	1622	CLA	C1C-NC-C4C	-4.39	104.58	107.05
14	A3	831	CLA	C1C-NC-C4C	-4.39	104.58	107.05
14	B2	829	CLA	C1C-NC-C4C	-4.36	104.60	107.05
14	A6	1631	CLA	C1C-NC-C4C	-4.33	104.61	107.05
14	A4	830	CLA	C1C-NC-C4C	-4.30	104.62	107.05
14	A1	830	CLA	C1C-NC-C4C	-4.29	104.63	107.05
14	A5	831	CLA	C1C-NC-C4C	-4.28	104.64	107.05
14	A4	819	CLA	C1C-NC-C4C	-4.22	104.67	107.05
14	A1	819	CLA	C1C-NC-C4C	-4.18	104.69	107.05
14	A3	820	CLA	C1C-NC-C4C	-4.15	104.71	107.05
14	B1	831	CLA	C1C-NC-C4C	-4.14	104.72	107.05
14	A5	820	CLA	C1C-NC-C4C	-4.13	104.72	107.05
14	A2	1622	CLA	C1C-NC-C4C	-4.13	104.72	107.05
15	B5	1844	PQN	C15-C13-C12	-4.10	112.75	121.10
15	B2	841	PQN	C15-C13-C12	-4.09	112.78	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B6	842	PQN	C15-C13-C12	-4.08	112.80	121.10
15	B4	844	PQN	C15-C13-C12	-4.08	112.80	121.10
14	A6	1620	CLA	C1C-NC-C4C	-4.07	104.75	107.05
14	A5	806	CLA	CAA-C2A-C3A	-4.07	101.66	112.81
14	A4	805	CLA	CAA-C2A-C3A	-4.04	101.74	112.81
14	A2	1608	CLA	CAA-C2A-C3A	-4.04	101.75	112.81
15	B3	1844	PQN	C15-C13-C12	-3.98	112.99	121.10
14	A6	1606	CLA	CAA-C2A-C3A	-3.97	101.92	112.81
14	A1	805	CLA	CAA-C2A-C3A	-3.97	101.93	112.81
15	B1	842	PQN	C15-C13-C12	-3.96	113.03	121.10
14	A3	806	CLA	CAA-C2A-C3A	-3.88	102.17	112.81
16	I5	102	BCR	C37-C22-C21	-3.76	117.66	122.92
16	B5	1847	BCR	C37-C22-C21	-3.68	117.78	122.92
16	B1	844	BCR	C34-C9-C10	-3.65	117.80	122.92
16	B3	1846	BCR	C34-C9-C10	-3.65	117.81	122.92
16	B5	1846	BCR	C34-C9-C10	-3.64	117.83	122.92
16	B2	844	BCR	C37-C22-C21	-3.64	117.83	122.92
16	B4	846	BCR	C34-C9-C10	-3.59	117.89	122.92
16	B4	847	BCR	C37-C22-C21	-3.59	117.89	122.92
16	L1	203	BCR	C37-C22-C21	-3.59	117.89	122.92
16	B6	845	BCR	C37-C22-C21	-3.58	117.91	122.92
16	B3	1847	BCR	C37-C22-C21	-3.57	117.92	122.92
16	B6	844	BCR	C34-C9-C10	-3.56	117.94	122.92
16	B1	845	BCR	C37-C22-C21	-3.55	117.95	122.92
16	I3	102	BCR	C37-C22-C21	-3.54	117.97	122.92
16	B2	843	BCR	C34-C9-C10	-3.51	118.00	122.92
16	L2	203	BCR	C37-C22-C21	-3.51	118.01	122.92
16	L6	204	BCR	C37-C22-C21	-3.46	118.07	122.92
16	I4	102	BCR	C37-C22-C21	-3.45	118.09	122.92
16	B5	1850	BCR	C12-C13-C14	-3.42	113.69	118.94
16	F4	201	BCR	C12-C13-C14	-3.39	113.74	118.94
16	B1	848	BCR	C12-C13-C14	-3.36	113.79	118.94
16	F6	201	BCR	C12-C13-C14	-3.31	113.86	118.94
16	F2	203	BCR	C35-C13-C14	-3.30	118.30	122.92
16	F4	203	BCR	C35-C13-C14	-3.29	118.31	122.92
16	F3	201	BCR	C12-C13-C14	-3.29	113.89	118.94
14	A4	818	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
16	F3	203	BCR	C35-C13-C14	-3.27	118.34	122.92
16	F2	201	BCR	C12-C13-C14	-3.26	113.93	118.94
14	B2	807	CLA	O1D-CGD-CBD	-3.26	118.53	124.58
14	A2	1621	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
16	F6	203	BCR	C35-C13-C14	-3.25	118.38	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	808	CLA	O1D-CGD-CBD	-3.21	118.62	124.58
16	F1	1302	BCR	C35-C13-C14	-3.20	118.44	122.92
16	F5	1302	BCR	C35-C13-C14	-3.19	118.45	122.92
14	A3	801	CLA	O2D-CGD-O1D	-3.19	117.49	123.82
14	B2	826	CLA	CHD-C4C-C3C	-3.14	120.25	124.88
14	A6	1621	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
14	A4	807	CLA	CHD-C4C-C3C	-3.13	120.27	124.88
16	B5	1846	BCR	C30-C25-C26	-3.12	118.20	122.59
14	A3	821	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
14	B1	802	CLA	O2A-CGA-O1A	-3.11	116.00	123.58
14	B1	819	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
14	A2	1610	CLA	CHD-C4C-C3C	-3.10	120.31	124.88
14	A6	1619	CLA	CMB-C2B-C1B	-3.08	123.74	128.46
14	A5	819	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
14	B1	810	CLA	O1D-CGD-CBD	-3.07	118.88	124.58
16	B1	848	BCR	C8-C9-C10	-3.07	114.23	118.94
14	B3	1820	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
14	B5	1829	CLA	CHD-C4C-C3C	-3.06	120.37	124.88
14	A6	1608	CLA	CHD-C4C-C3C	-3.05	120.38	124.88
14	A3	819	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
14	B4	810	CLA	O1D-CGD-CBD	-3.04	118.94	124.58
14	B4	820	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
16	F4	201	BCR	C8-C9-C10	-3.04	114.28	118.94
14	B6	827	CLA	CHD-C4C-C3C	-3.03	120.40	124.88
14	A2	1604	CLA	O2A-CGA-O1A	-3.02	116.20	123.58
14	B1	853	CLA	CHD-C4C-C3C	-3.02	120.42	124.88
16	B3	1846	BCR	C30-C25-C26	-3.02	118.35	122.59
14	B2	817	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
14	B6	818	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
14	B1	828	CLA	CHD-C4C-C3C	-3.01	120.44	124.88
14	B5	1810	CLA	O1D-CGD-CBD	-3.01	119.00	124.58
16	B1	844	BCR	C30-C25-C26	-3.01	118.37	122.59
16	B1	844	BCR	C1-C6-C5	-3.00	118.37	122.59
14	A5	808	CLA	CHD-C4C-C3C	-3.00	120.45	124.88
14	A1	807	CLA	CHD-C4C-C3C	-3.00	120.46	124.88
14	B4	829	CLA	CHD-C4C-C3C	-3.00	120.46	124.88
14	A5	821	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
14	A3	808	CLA	CHD-C4C-C3C	-2.99	120.47	124.88
16	B5	1850	BCR	C8-C9-C10	-2.98	114.36	118.94
14	A1	818	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
14	A5	841	CLA	CHD-C4C-C3C	-2.98	120.49	124.88
16	B2	843	BCR	C30-C25-C26	-2.98	118.41	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A1	801	CLA	O2D-CGD-O1D	-2.97	117.92	123.82
14	A2	1623	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
14	B3	1804	CLA	O2D-CGD-O1D	-2.97	117.93	123.82
14	B3	1829	CLA	CHD-C4C-C3C	-2.97	120.50	124.88
16	B4	846	BCR	C30-C25-C26	-2.96	118.43	122.59
14	A1	838	CLA	CHD-C4C-C3C	-2.95	120.52	124.88
14	A1	820	CLA	CMB-C2B-C1B	-2.95	123.92	128.46
14	B3	1810	CLA	O1D-CGD-CBD	-2.95	119.10	124.58
14	B3	1817	CLA	CHD-C4C-C3C	-2.95	120.53	124.88
14	A4	820	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
14	A1	825	CLA	CHD-C4C-C3C	-2.95	120.53	124.88
14	A5	843	CLA	CHD-C4C-C3C	-2.95	120.53	124.88
14	A4	840	CLA	CHD-C4C-C3C	-2.94	120.54	124.88
16	B6	844	BCR	C30-C25-C26	-2.94	118.46	122.59
14	A6	1640	CLA	CHD-C4C-C3C	-2.93	120.56	124.88
16	F2	201	BCR	C8-C9-C10	-2.93	114.45	118.94
14	A5	836	CLA	O2A-CGA-O1A	-2.93	116.44	123.58
14	A6	1651	CLA	O2D-CGD-O1D	-2.92	118.02	123.82
14	B1	810	CLA	O2A-CGA-O1A	-2.92	116.45	123.58
14	B5	1811	CLA	CBC-CAC-C3C	-2.92	104.29	112.42
14	B3	1811	CLA	CBC-CAC-C3C	-2.92	104.29	112.42
14	B2	808	CLA	CBC-CAC-C3C	-2.92	104.29	112.42
14	A5	801	CLA	O2D-CGD-O1D	-2.91	118.03	123.82
14	A6	1604	CLA	O1D-CGD-CBD	-2.91	119.18	124.58
14	L5	203	CLA	O1D-CGD-CBD	-2.91	119.18	124.58
14	B5	1801	CLA	CHD-C4C-C3C	-2.91	120.59	124.88
14	B5	1827	CLA	O1D-CGD-CBD	-2.91	119.19	124.58
14	B1	816	CLA	CHD-C4C-C3C	-2.90	120.60	124.88
14	B4	852	CLA	CHD-C4C-C3C	-2.90	120.60	124.88
14	B4	802	CLA	O2A-CGA-O1A	-2.90	116.50	123.58
14	B5	1820	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
14	A2	1602	CLA	O2D-CGD-O1D	-2.90	118.07	123.82
14	A5	826	CLA	CHD-C4C-C3C	-2.90	120.61	124.88
14	B5	1817	CLA	CHD-C4C-C3C	-2.90	120.61	124.88
14	B5	1810	CLA	O2A-CGA-O1A	-2.90	116.52	123.58
14	A1	834	CLA	O2A-CGA-O1A	-2.89	116.52	123.58
14	B3	1801	CLA	CHD-C4C-C3C	-2.89	120.61	124.88
14	A2	1643	CLA	CHD-C4C-C3C	-2.89	120.61	124.88
16	B6	844	BCR	C1-C6-C5	-2.89	118.53	122.59
16	M4	101	BCR	C1-C6-C5	-2.89	118.53	122.59
14	A3	845	CLA	CHD-C4C-C3C	-2.89	120.62	124.88
16	B5	1846	BCR	C1-C6-C5	-2.89	118.53	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B2	824	CLA	O1D-CGD-CBD	-2.88	119.24	124.58
16	B3	1846	BCR	C1-C6-C5	-2.88	118.55	122.59
14	A4	801	CLA	O2D-CGD-O1D	-2.88	118.11	123.82
14	A6	1633	CLA	O1D-CGD-CBD	-2.88	119.25	124.58
14	B3	1802	CLA	O2A-CGA-O1A	-2.87	116.57	123.58
14	B1	811	CLA	CBC-CAC-C3C	-2.87	104.42	112.42
16	M2	1202	BCR	C1-C6-C5	-2.87	118.55	122.59
16	B6	850	BCR	C1-C6-C5	-2.87	118.56	122.59
16	A4	849	BCR	C23-C22-C21	-2.87	114.54	118.94
14	A3	837	CLA	O2A-CGA-O1A	-2.87	116.58	123.58
14	A6	1603	CLA	O2A-CGA-O1A	-2.87	116.58	123.58
14	B6	815	CLA	CHD-C4C-C3C	-2.87	120.65	124.88
14	B5	1802	CLA	O2A-CGA-O1A	-2.87	116.59	123.58
14	A3	834	CLA	O1D-CGD-CBD	-2.86	119.27	124.58
14	B2	814	CLA	CHD-C4C-C3C	-2.86	120.66	124.88
14	A2	1644	CLA	O2A-CGA-O1A	-2.86	116.60	123.58
14	L2	205	CLA	CHD-C4C-C3C	-2.86	120.66	124.88
14	A2	1606	CLA	O1D-CGD-CBD	-2.86	119.28	124.58
14	B4	811	CLA	CBC-CAC-C3C	-2.86	104.47	112.42
14	B4	817	CLA	CHD-C4C-C3C	-2.86	120.67	124.88
14	L3	203	CLA	O1D-CGD-CBD	-2.85	119.28	124.58
16	J5	105	BCR	C1-C6-C5	-2.85	118.58	122.59
14	A5	804	CLA	O1D-CGD-CBD	-2.85	119.30	124.58
16	B3	1851	BCR	C1-C6-C5	-2.84	118.61	122.59
16	B2	843	BCR	C1-C6-C5	-2.83	118.61	122.59
14	B6	825	CLA	O1D-CGD-CBD	-2.83	119.33	124.58
14	B3	1831	CLA	O1D-CGD-CBD	-2.83	119.33	124.58
14	A1	839	CLA	O2A-CGA-O1A	-2.83	116.68	123.58
16	M1	1202	BCR	C1-C6-C5	-2.83	118.62	122.59
16	F3	201	BCR	C8-C9-C10	-2.83	114.60	118.94
14	B6	809	CLA	CBC-CAC-C3C	-2.83	104.55	112.42
16	A5	849	BCR	C38-C26-C27	-2.83	108.22	113.56
14	A2	1609	CLA	CHD-C4C-C3C	-2.82	120.72	124.88
14	B1	834	CLA	O1D-CGD-CBD	-2.82	119.35	124.58
14	A5	807	CLA	CHD-C4C-C3C	-2.82	120.72	124.88
14	A5	831	CLA	O1D-CGD-CBD	-2.82	119.35	124.58
14	B3	1801	CLA	O1D-CGD-CBD	-2.82	119.36	124.58
14	A2	1638	CLA	O2A-CGA-O1A	-2.82	116.71	123.58
14	A3	826	CLA	CHD-C4C-C3C	-2.81	120.73	124.88
16	F4	204	BCR	C1-C6-C5	-2.81	118.64	122.59
14	A6	1602	CLA	O2D-CGD-O1D	-2.81	118.25	123.82
14	B5	1801	CLA	O1D-CGD-CBD	-2.81	119.38	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	810	CLA	O2A-CGA-O1A	-2.81	116.73	123.58
14	A4	837	CLA	O2A-CGA-O1A	-2.80	116.74	123.58
16	I4	102	BCR	C33-C5-C4	-2.80	108.26	113.56
14	A6	1639	CLA	CHD-C4C-C3C	-2.80	120.74	124.88
16	A6	1647	BCR	C38-C26-C27	-2.80	108.27	113.56
14	A4	835	CLA	O2A-CGA-O1A	-2.80	116.75	123.58
16	A2	1651	BCR	C38-C26-C27	-2.80	108.28	113.56
16	B2	842	BCR	C38-C26-C27	-2.79	108.28	113.56
14	A3	842	CLA	CHD-C4C-C3C	-2.79	120.76	124.88
14	B3	1827	CLA	O1D-CGD-CBD	-2.79	119.40	124.58
14	B2	812	CLA	O1D-CGD-CBD	-2.79	119.40	124.58
14	B1	830	CLA	O1D-CGD-CBD	-2.79	119.40	124.58
14	B6	808	CLA	O2A-CGA-O1A	-2.79	116.77	123.58
16	F6	201	BCR	C8-C9-C10	-2.79	114.66	118.94
14	M6	1201	CLA	CHD-C4C-C3C	-2.79	120.77	124.88
14	B6	815	CLA	O1D-CGD-CBD	-2.78	119.42	124.58
16	B5	1845	BCR	C38-C26-C27	-2.78	108.30	113.56
14	A3	804	CLA	O1D-CGD-CBD	-2.78	119.42	124.58
16	B2	850	BCR	C1-C6-C5	-2.78	118.68	122.59
14	L6	206	CLA	CHD-C4C-C3C	-2.78	120.78	124.88
16	A6	1648	BCR	C23-C22-C21	-2.78	114.68	118.94
14	B3	1835	CLA	O1D-CGD-CBD	-2.78	119.43	124.58
14	M1	1201	CLA	CHD-C4C-C3C	-2.78	120.78	124.88
14	B4	835	CLA	O1D-CGD-CBD	-2.78	119.43	124.58
14	A3	845	CLA	O1D-CGD-CBD	-2.77	119.44	124.58
16	B4	845	BCR	C38-C26-C27	-2.77	108.33	113.56
14	L3	203	CLA	CHD-C4C-C3C	-2.77	120.79	124.88
14	L1	202	CLA	CHD-C4C-C3C	-2.77	120.79	124.88
14	B6	814	CLA	O1D-CGD-CBD	-2.77	119.45	124.58
16	M6	1202	BCR	C1-C6-C5	-2.77	118.70	122.59
17	A5	852	LHG	C6-C5-C4	-2.76	105.62	111.86
14	A6	1636	CLA	O2A-CGA-O1A	-2.76	116.84	123.58
14	B4	828	CLA	CHD-C4C-C3C	-2.76	120.81	124.88
16	A3	851	BCR	C38-C26-C27	-2.76	108.35	113.56
14	B3	1810	CLA	O2A-CGA-O1A	-2.76	116.85	123.58
14	B3	1816	CLA	O1D-CGD-CBD	-2.76	119.47	124.58
14	A5	842	CLA	O2A-CGA-O1A	-2.75	116.86	123.58
14	B1	805	CLA	O2D-CGD-O1D	-2.75	118.37	123.82
14	A4	838	CLA	CHD-C4C-C3C	-2.75	120.83	124.88
14	B1	832	CLA	CHD-C4C-C3C	-2.75	120.83	124.88
14	B5	1835	CLA	O1D-CGD-CBD	-2.74	119.49	124.58
16	A3	852	BCR	C23-C22-C21	-2.74	114.73	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B4	846	BCR	C1-C6-C5	-2.74	118.74	122.59
14	A6	1638	CLA	O2A-CGA-O1A	-2.74	116.89	123.58
14	B1	803	CLA	CHD-C4C-C3C	-2.74	120.84	124.88
14	A6	1617	CLA	CHD-C4C-C3C	-2.73	120.85	124.88
16	B1	843	BCR	C38-C26-C27	-2.73	108.39	113.56
14	L1	202	CLA	O1D-CGD-CBD	-2.73	119.51	124.58
14	L4	201	CLA	O1D-CGD-CBD	-2.73	119.52	124.58
14	A4	806	CLA	CHD-C4C-C3C	-2.73	120.85	124.88
14	B2	832	CLA	O1D-CGD-CBD	-2.73	119.52	124.58
17	A1	849	LHG	C6-C5-C4	-2.73	105.70	111.86
16	M5	101	BCR	C1-C6-C5	-2.73	118.76	122.59
14	A2	1640	CLA	O2A-CGA-O1A	-2.73	116.93	123.58
14	B2	813	CLA	O1D-CGD-CBD	-2.73	119.52	124.58
16	B1	852	BCR	C1-C6-C5	-2.73	118.76	122.59
16	B3	1851	BCR	C33-C5-C4	-2.72	108.41	113.56
14	B1	838	CLA	CHD-C4C-C3C	-2.72	120.86	124.88
14	A2	1628	CLA	CHD-C4C-C3C	-2.72	120.86	124.88
14	L1	205	CLA	O1D-CGD-CBD	-2.72	119.53	124.58
14	B5	1806	CLA	CHD-C4C-C3C	-2.72	120.87	124.88
14	A3	807	CLA	CHD-C4C-C3C	-2.72	120.87	124.88
14	B6	826	CLA	CHD-C4C-C3C	-2.72	120.87	124.88
14	B6	830	CLA	O1D-CGD-CBD	-2.72	119.54	124.58
16	A4	848	BCR	C38-C26-C27	-2.72	108.43	113.56
16	A1	846	BCR	C38-C26-C27	-2.72	108.43	113.56
17	A4	851	LHG	C6-C5-C4	-2.72	105.73	111.86
14	A1	806	CLA	CHD-C4C-C3C	-2.71	120.87	124.88
14	A2	1642	CLA	CHD-C4C-C3C	-2.71	120.88	124.88
14	B2	807	CLA	O2A-CGA-O1A	-2.71	116.96	123.58
14	A6	1626	CLA	CHD-C4C-C3C	-2.71	120.88	124.88
14	A4	825	CLA	CHD-C4C-C3C	-2.71	120.88	124.88
14	A3	817	CLA	CHD-C4C-C3C	-2.71	120.89	124.88
14	A5	811	CLA	CHD-C4C-C3C	-2.71	120.89	124.88
14	L5	203	CLA	CHD-C4C-C3C	-2.71	120.89	124.88
16	A2	1652	BCR	C23-C22-C21	-2.71	114.79	118.94
14	A5	843	CLA	O1D-CGD-CBD	-2.71	119.56	124.58
14	B5	1811	CLA	CHD-C4C-C3C	-2.70	120.89	124.88
14	B4	827	CLA	O1D-CGD-CBD	-2.70	119.56	124.58
14	A3	841	CLA	CHD-C4C-C3C	-2.70	120.89	124.88
14	L1	205	CLA	CHD-C4C-C3C	-2.70	120.89	124.88
14	L5	204	CLA	O1D-CGD-CBD	-2.70	119.57	124.58
16	B4	845	BCR	C1-C6-C5	-2.70	118.79	122.59
14	B3	1828	CLA	CHD-C4C-C3C	-2.70	120.89	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	810	CLA	CHD-C4C-C3C	-2.70	120.89	124.88
17	A6	1650	LHG	C6-C5-C4	-2.70	105.76	111.86
14	A4	839	CLA	CHD-C4C-C3C	-2.70	120.90	124.88
14	A5	817	CLA	CHD-C4C-C3C	-2.70	120.90	124.88
14	B5	1804	CLA	O2D-CGD-O1D	-2.70	118.47	123.82
14	A3	843	CLA	O2A-CGA-O1A	-2.70	117.00	123.58
14	A6	1635	CLA	CHD-C4C-C3C	-2.70	120.90	124.88
14	A1	816	CLA	CHD-C4C-C3C	-2.69	120.90	124.88
14	B5	1823	CLA	O1D-CGD-CBD	-2.69	119.58	124.58
14	B6	833	CLA	O1D-CGD-CBD	-2.69	119.59	124.58
14	B6	813	CLA	O1D-CGD-CBD	-2.69	119.59	124.58
14	A5	839	CLA	CHD-C4C-C3C	-2.69	120.91	124.88
16	B3	1845	BCR	C38-C26-C27	-2.69	108.48	113.56
14	A6	1633	CLA	CHD-C4C-C3C	-2.69	120.92	124.88
16	A3	847	BCR	C30-C25-C26	-2.69	118.82	122.59
14	A2	1641	CLA	CHD-C4C-C3C	-2.68	120.92	124.88
16	I3	102	BCR	C33-C5-C4	-2.68	108.49	113.56
14	A6	1631	CLA	O1D-CGD-CBD	-2.68	119.61	124.58
14	B2	836	CLA	CHD-C4C-C3C	-2.68	120.92	124.88
14	A5	840	CLA	CHD-C4C-C3C	-2.68	120.92	124.88
14	B4	831	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
14	A3	834	CLA	CHD-C4C-C3C	-2.68	120.92	124.88
14	L5	204	CLA	CHD-C4C-C3C	-2.68	120.92	124.88
14	A3	840	CLA	CHD-C4C-C3C	-2.68	120.92	124.88
16	A2	1652	BCR	C36-C18-C17	-2.68	119.17	122.92
16	B6	843	BCR	C38-C26-C27	-2.68	108.50	113.56
16	B3	1845	BCR	C1-C6-C5	-2.68	118.83	122.59
14	A1	805	CLA	O2A-CGA-O1A	-2.68	117.05	123.58
14	A3	830	CLA	CHD-C4C-C3C	-2.68	120.93	124.88
14	A3	837	CLA	CHD-C4C-C3C	-2.68	120.93	124.88
14	A4	807	CLA	O1D-CGD-CBD	-2.68	119.62	124.58
14	B2	828	CLA	CMB-C2B-C1B	-2.67	124.35	128.46
14	A1	830	CLA	O1D-CGD-CBD	-2.67	119.62	124.58
14	B5	1803	CLA	C7-C6-C5	-2.67	105.90	113.17
17	A3	854	LHG	C6-C5-C4	-2.67	105.83	111.86
14	B4	852	CLA	O1D-CGD-CBD	-2.67	119.62	124.58
16	L2	203	BCR	C19-C18-C17	-2.67	114.84	118.94
14	B6	803	CLA	CHD-C4C-C3C	-2.67	120.94	124.88
14	A4	803	CLA	O1D-CGD-CBD	-2.67	119.63	124.58
16	A5	850	BCR	C23-C22-C21	-2.67	114.85	118.94
14	B4	804	CLA	C1C-C2C-C3C	-2.67	104.08	106.93
14	L4	203	CLA	CHD-C4C-C3C	-2.67	120.95	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B3	1847	BCR	C1-C6-C5	-2.66	118.85	122.59
16	L6	204	BCR	C33-C5-C4	-2.66	108.53	113.56
14	B4	803	CLA	C7-C6-C5	-2.66	105.92	113.17
14	A2	1633	CLA	O1D-CGD-CBD	-2.66	119.64	124.58
14	B5	1813	CLA	CHD-C4C-C3C	-2.66	120.95	124.88
16	B5	1846	BCR	C38-C26-C27	-2.66	108.53	113.56
14	A6	1636	CLA	CHD-C4C-C3C	-2.66	120.96	124.88
14	B3	1804	CLA	CHD-C4C-C3C	-2.66	120.96	124.88
14	A5	838	CLA	O2A-CGA-O1A	-2.66	117.10	123.58
14	B1	830	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
14	B6	808	CLA	CHD-C4C-C3C	-2.65	120.98	124.88
14	A4	841	CLA	O2A-CGA-O1A	-2.64	117.13	123.58
16	B2	842	BCR	C1-C6-C5	-2.64	118.88	122.59
14	B5	1831	CLA	O1D-CGD-CBD	-2.64	119.68	124.58
14	B4	833	CLA	CHD-C4C-C3C	-2.64	120.98	124.88
14	A3	828	CLA	CHD-C4C-C3C	-2.64	120.98	124.88
14	B4	831	CLA	O1D-CGD-CBD	-2.64	119.68	124.58
14	A6	1607	CLA	CHD-C4C-C3C	-2.64	120.98	124.88
14	B5	1833	CLA	CHD-C4C-C3C	-2.64	120.98	124.88
14	B3	1807	CLA	CHD-C4C-C3C	-2.64	120.98	124.88
14	A2	1631	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
14	A4	816	CLA	CHD-C4C-C3C	-2.64	120.99	124.88
16	I4	102	BCR	C19-C18-C17	-2.64	114.89	118.94
14	A6	1651	CLA	CHD-C4C-C3C	-2.64	120.99	124.88
14	A5	825	CLA	O1D-CGD-CBD	-2.63	119.70	124.58
16	B6	843	BCR	C30-C25-C26	-2.63	118.89	122.59
14	B4	804	CLA	O1D-CGD-CBD	-2.63	119.70	124.58
14	A1	828	CLA	CHD-C4C-C3C	-2.63	121.00	124.88
16	M3	1602	BCR	C1-C6-C5	-2.63	118.90	122.59
14	A3	836	CLA	CHD-C4C-C3C	-2.63	121.00	124.88
14	B4	804	CLA	O2D-CGD-O1D	-2.63	118.60	123.82
16	L3	206	BCR	C33-C5-C4	-2.63	108.60	113.56
14	B1	812	CLA	CHD-C4C-C3C	-2.63	121.01	124.88
16	I1	103	BCR	C33-C5-C4	-2.62	108.60	113.56
14	B2	828	CLA	O1D-CGD-CBD	-2.62	119.72	124.58
16	L2	208	BCR	C33-C5-C4	-2.62	108.61	113.56
14	B1	805	CLA	C1C-C2C-C3C	-2.62	104.12	106.93
14	B1	827	CLA	CHD-C4C-C3C	-2.62	121.02	124.88
14	L6	203	CLA	CHD-C4C-C3C	-2.62	121.02	124.88
14	A2	1610	CLA	O1D-CGD-CBD	-2.62	119.72	124.58
16	B6	845	BCR	C1-C6-C5	-2.62	118.91	122.59
14	B4	806	CLA	CHD-C4C-C3C	-2.62	121.02	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B2	840	CLA	CHD-C4C-C3C	-2.62	121.02	124.88
14	A6	1606	CLA	O2A-CGA-O1A	-2.62	117.20	123.58
14	L4	203	CLA	O1D-CGD-CBD	-2.62	119.73	124.58
14	B2	804	CLA	CHD-C4C-C3C	-2.61	121.03	124.88
14	B6	811	CLA	CHD-C4C-C3C	-2.61	121.03	124.88
14	B3	1806	CLA	O1D-CGD-CBD	-2.61	119.74	124.58
14	B1	816	CLA	O1D-CGD-CBD	-2.61	119.74	124.58
14	A3	801	CLA	CHD-C4C-C3C	-2.61	121.03	124.88
14	M2	1201	CLA	CHD-C4C-C3C	-2.61	121.03	124.88
16	L2	203	BCR	C33-C5-C4	-2.61	108.63	113.56
14	A1	809	CLA	CHD-C4C-C3C	-2.61	121.03	124.88
16	F6	201	BCR	C33-C5-C4	-2.61	108.63	113.56
14	A6	1628	CLA	CHD-C4C-C3C	-2.61	121.03	124.88
14	A4	834	CLA	CHD-C4C-C3C	-2.60	121.04	124.88
16	B1	848	BCR	C33-C5-C4	-2.60	108.64	113.56
14	A5	835	CLA	CHD-C4C-C3C	-2.60	121.04	124.88
14	A6	1630	CLA	CHD-C4C-C3C	-2.60	121.04	124.88
14	B6	806	CLA	CHD-C4C-C3C	-2.60	121.04	124.88
16	F3	201	BCR	C33-C5-C4	-2.60	108.64	113.56
14	B5	1816	CLA	O1D-CGD-CBD	-2.60	119.75	124.58
14	A1	837	CLA	CHD-C4C-C3C	-2.60	121.04	124.88
16	B1	843	BCR	C30-C25-C26	-2.60	118.94	122.59
14	B5	1804	CLA	CHD-C4C-C3C	-2.60	121.05	124.88
16	A4	844	BCR	C1-C6-C5	-2.60	118.94	122.59
14	A6	1608	CLA	O1D-CGD-CBD	-2.60	119.76	124.58
14	B6	837	CLA	CHD-C4C-C3C	-2.60	121.05	124.88
14	A5	840	CLA	O2A-CGA-O1A	-2.60	117.25	123.58
14	A1	836	CLA	O2A-CGA-O1A	-2.60	117.25	123.58
16	L4	206	BCR	C33-C5-C4	-2.60	108.66	113.56
14	A1	810	CLA	CHD-C4C-C3C	-2.60	121.05	124.88
16	A2	1647	BCR	C1-C6-C5	-2.60	118.94	122.59
14	A4	829	CLA	CHD-C4C-C3C	-2.60	121.05	124.88
16	B4	846	BCR	C38-C26-C27	-2.59	108.66	113.56
14	B1	841	CLA	CHD-C4C-C3C	-2.59	121.05	124.88
14	A2	1619	CLA	CHD-C4C-C3C	-2.59	121.05	124.88
16	J5	103	BCR	C30-C25-C26	-2.59	118.94	122.59
14	A3	829	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
14	B3	1833	CLA	CHD-C4C-C3C	-2.59	121.06	124.88
14	A3	811	CLA	CHD-C4C-C3C	-2.59	121.06	124.88
14	A5	830	CLA	CHD-C4C-C3C	-2.59	121.06	124.88
14	B5	1810	CLA	CHD-C4C-C3C	-2.59	121.06	124.88
14	B3	1811	CLA	CHD-C4C-C3C	-2.59	121.06	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A5	829	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
14	B3	1810	CLA	CHD-C4C-C3C	-2.59	121.06	124.88
14	B3	1812	CLA	C1C-C2C-C3C	-2.59	104.16	106.93
14	B3	1839	CLA	CHD-C4C-C3C	-2.59	121.06	124.88
14	A5	806	CLA	O2A-CGA-O1A	-2.59	117.27	123.58
14	B3	1813	CLA	CHD-C4C-C3C	-2.59	121.06	124.88
14	B3	1815	CLA	O1D-CGD-CBD	-2.59	119.78	124.58
14	B4	815	CLA	O1D-CGD-CBD	-2.58	119.79	124.58
14	B3	1825	CLA	CHD-C4C-C3C	-2.58	121.07	124.88
14	B3	1837	CLA	CHD-C4C-C3C	-2.58	121.07	124.88
14	B2	829	CLA	O1D-CGD-CBD	-2.58	119.79	124.58
14	A3	839	CLA	O2A-CGA-O1A	-2.58	117.28	123.58
14	B6	829	CLA	O1D-CGD-CBD	-2.58	119.79	124.58
14	A1	815	CLA	CHD-C4C-C3C	-2.58	121.07	124.88
16	A3	847	BCR	C1-C6-C5	-2.58	118.97	122.59
14	A3	827	CLA	O1D-CGD-CBD	-2.58	119.80	124.58
14	B2	807	CLA	CHD-C4C-C3C	-2.58	121.08	124.88
16	A4	845	BCR	C1-C6-C5	-2.58	118.97	122.59
14	B2	801	CLA	C7-C6-C5	-2.58	106.16	113.17
14	B2	802	CLA	O1D-CGD-CBD	-2.58	119.80	124.58
14	A3	843	CLA	CHD-C4C-C3C	-2.58	121.08	124.88
16	I3	102	BCR	C19-C18-C17	-2.58	114.99	118.94
14	A2	1632	CLA	CHD-C4C-C3C	-2.57	121.08	124.88
14	B3	1817	CLA	O1D-CGD-CBD	-2.57	119.81	124.58
14	A4	828	CLA	CMB-C2B-C1B	-2.57	124.51	128.46
14	B1	817	CLA	CHD-C4C-C3C	-2.57	121.09	124.88
16	A1	847	BCR	C23-C22-C21	-2.57	115.00	118.94
14	B5	1817	CLA	O1D-CGD-CBD	-2.57	119.81	124.58
16	I5	102	BCR	C33-C5-C4	-2.57	108.71	113.56
14	A3	815	CLA	O1D-CGD-CBD	-2.57	119.82	124.58
14	B5	1828	CLA	CHD-C4C-C3C	-2.57	121.09	124.88
16	A5	845	BCR	C1-C6-C5	-2.57	118.99	122.59
14	A1	803	CLA	O1D-CGD-CBD	-2.56	119.82	124.58
14	B5	1831	CLA	CMB-C2B-C1B	-2.56	124.52	128.46
14	B2	802	CLA	O2D-CGD-O1D	-2.56	118.73	123.82
14	B5	1843	CLA	CHD-C4C-C3C	-2.56	121.10	124.88
16	B4	845	BCR	C30-C25-C26	-2.56	118.99	122.59
14	A2	1608	CLA	O2A-CGA-O1A	-2.56	117.33	123.58
14	A1	833	CLA	CHD-C4C-C3C	-2.56	121.10	124.88
14	B3	1802	CLA	CBC-CAC-C3C	-2.56	105.29	112.42
14	B1	853	CLA	O1D-CGD-CBD	-2.56	119.83	124.58
16	F2	201	BCR	C33-C5-C4	-2.56	108.72	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B3	1822	CLA	O1D-CGD-CBD	-2.56	119.83	124.58
14	L2	205	CLA	O1D-CGD-CBD	-2.56	119.83	124.58
14	A6	1618	CLA	CHD-C4C-C3C	-2.56	121.10	124.88
14	B1	826	CLA	O1D-CGD-CBD	-2.56	119.83	124.58
14	A2	1620	CLA	CHD-C4C-C3C	-2.56	121.11	124.88
16	L6	204	BCR	C19-C18-C17	-2.56	115.02	118.94
14	A4	805	CLA	O2A-CGA-O1A	-2.56	117.34	123.58
16	A4	846	BCR	C1-C6-C5	-2.56	119.00	122.59
14	A1	824	CLA	CHD-C4C-C3C	-2.56	121.11	124.88
14	A6	1611	CLA	CHD-C4C-C3C	-2.56	121.11	124.88
14	A4	824	CLA	CHD-C4C-C3C	-2.56	121.11	124.88
14	M3	1601	CLA	CHD-C4C-C3C	-2.56	121.11	124.88
14	L6	206	CLA	O1D-CGD-CBD	-2.56	119.84	124.58
14	B3	1838	CLA	CHD-C4C-C3C	-2.56	121.11	124.88
14	A4	801	CLA	CHD-C4C-C3C	-2.55	121.11	124.88
16	F4	201	BCR	C33-C5-C4	-2.55	108.73	113.56
14	L6	203	CLA	O2A-CGA-O1A	-2.55	117.35	123.58
16	B3	1847	BCR	C34-C9-C10	-2.55	119.35	122.92
16	A1	844	BCR	C1-C6-C5	-2.55	119.00	122.59
14	B2	809	CLA	C1C-C2C-C3C	-2.55	104.20	106.93
14	A5	828	CLA	CHD-C4C-C3C	-2.55	121.11	124.88
14	A2	1612	CLA	CHD-C4C-C3C	-2.55	121.12	124.88
16	F4	204	BCR	C33-C5-C4	-2.55	108.74	113.56
14	L2	202	CLA	CHD-C4C-C3C	-2.55	121.12	124.88
14	A2	1638	CLA	CHD-C4C-C3C	-2.55	121.12	124.88
16	B6	845	BCR	C34-C9-C10	-2.55	119.35	122.92
14	A5	842	CLA	CHD-C4C-C3C	-2.55	121.12	124.88
14	L4	201	CLA	CHD-C4C-C3C	-2.55	121.12	124.88
14	A1	826	CLA	O1D-CGD-CBD	-2.55	119.85	124.58
14	A3	827	CLA	CHD-C4C-C3C	-2.55	121.12	124.88
16	B1	852	BCR	C33-C5-C4	-2.55	108.75	113.56
14	B4	821	CLA	CHD-C4C-C3C	-2.54	121.13	124.88
16	I1	102	BCR	C19-C18-C17	-2.54	115.04	118.94
14	B5	1839	CLA	CHD-C4C-C3C	-2.54	121.13	124.88
16	B6	843	BCR	C1-C6-C5	-2.54	119.02	122.59
14	B6	810	CLA	C1C-C2C-C3C	-2.54	104.21	106.93
14	B4	807	CLA	CHD-C4C-C3C	-2.54	121.13	124.88
14	B2	808	CLA	CHD-C4C-C3C	-2.54	121.13	124.88
14	A6	1601	CLA	CHD-C4C-C3C	-2.54	121.13	124.88
14	B4	816	CLA	O1D-CGD-CBD	-2.54	119.87	124.58
14	B1	815	CLA	O1D-CGD-CBD	-2.54	119.87	124.58
14	B4	812	CLA	C1C-C2C-C3C	-2.54	104.21	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A5	816	CLA	CHD-C4C-C3C	-2.54	121.13	124.88
16	L1	203	BCR	C33-C5-C4	-2.54	108.76	113.56
16	J5	105	BCR	C33-C5-C4	-2.54	108.76	113.56
16	B1	845	BCR	C34-C9-C10	-2.54	119.37	122.92
14	B1	804	CLA	C7-C6-C5	-2.54	106.27	113.17
14	A4	830	CLA	O1D-CGD-CBD	-2.54	119.87	124.58
14	B4	813	CLA	CHD-C4C-C3C	-2.54	121.14	124.88
14	B2	814	CLA	O1D-CGD-CBD	-2.54	119.87	124.58
14	A6	1629	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
14	L5	202	CLA	CHD-C4C-C3C	-2.54	121.14	124.88
16	A6	1643	BCR	C30-C25-C26	-2.54	119.03	122.59
14	B4	810	CLA	CHD-C4C-C3C	-2.54	121.14	124.88
14	A4	817	CLA	CHD-C4C-C3C	-2.54	121.14	124.88
16	B3	1849	BCR	C33-C5-C4	-2.53	108.77	113.56
14	A4	828	CLA	CHD-C4C-C3C	-2.53	121.14	124.88
14	B3	1806	CLA	CHD-C4C-C3C	-2.53	121.14	124.88
16	L5	207	BCR	C33-C5-C4	-2.53	108.77	113.56
14	B2	835	CLA	CHD-C4C-C3C	-2.53	121.14	124.88
14	B1	854	CLA	C1C-C2C-C3C	-2.53	104.22	106.93
14	B6	820	CLA	O1D-CGD-CBD	-2.53	119.88	124.58
16	L6	209	BCR	C33-C5-C4	-2.53	108.78	113.56
14	A5	820	CLA	CHD-C4C-C3C	-2.53	121.14	124.88
16	A2	1649	BCR	C1-C6-C5	-2.53	119.03	122.59
14	B3	1831	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
16	B5	1845	BCR	C1-C6-C5	-2.53	119.03	122.59
14	A1	828	CLA	CMB-C2B-C1B	-2.53	124.58	128.46
16	B5	1845	BCR	C30-C25-C26	-2.53	119.04	122.59
16	B5	1847	BCR	C34-C9-C10	-2.53	119.38	122.92
16	B2	842	BCR	C30-C25-C26	-2.52	119.04	122.59
14	L2	202	CLA	O1D-CGD-CBD	-2.52	119.90	124.58
14	A4	835	CLA	CHD-C4C-C3C	-2.52	121.16	124.88
14	B6	816	CLA	CHD-C4C-C3C	-2.52	121.16	124.88
16	A6	1645	BCR	C1-C6-C5	-2.52	119.05	122.59
16	B3	1845	BCR	C30-C25-C26	-2.52	119.05	122.59
16	A5	845	BCR	C30-C25-C26	-2.52	119.05	122.59
14	A2	1627	CLA	CHD-C4C-C3C	-2.52	121.16	124.88
16	I5	102	BCR	C19-C18-C17	-2.52	115.07	118.94
14	B1	805	CLA	O2A-CGA-O1A	-2.52	117.43	123.58
14	A2	1611	CLA	CHD-C4C-C3C	-2.52	121.16	124.88
14	A1	827	CLA	CHD-C4C-C3C	-2.52	121.16	124.88
14	B1	807	CLA	CHD-C4C-C3C	-2.52	121.16	124.88
16	B2	850	BCR	C33-C5-C4	-2.52	108.80	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	843	CLA	CHD-C4C-C3C	-2.52	121.16	124.88
14	A1	817	CLA	CHD-C4C-C3C	-2.52	121.17	124.88
14	B4	839	CLA	CHD-C4C-C3C	-2.52	121.17	124.88
14	B2	838	CLA	CHD-C4C-C3C	-2.52	121.17	124.88
14	A5	818	CLA	CHD-C4C-C3C	-2.52	121.17	124.88
14	B6	839	CLA	CHD-C4C-C3C	-2.52	121.17	124.88
14	A6	1625	CLA	O1D-CGD-CBD	-2.52	119.91	124.58
14	A1	834	CLA	CHD-C4C-C3C	-2.52	121.17	124.88
14	B2	820	CLA	O1D-CGD-CBD	-2.52	119.91	124.58
14	B6	831	CLA	CHD-C4C-C3C	-2.52	121.17	124.88
14	B1	840	CLA	CHD-C4C-C3C	-2.52	121.17	124.88
14	A5	829	CLA	CHD-C4C-C3C	-2.51	121.17	124.88
14	A2	1637	CLA	CHD-C4C-C3C	-2.51	121.17	124.88
14	A2	1631	CLA	CHD-C4C-C3C	-2.51	121.17	124.88
14	A2	1622	CLA	CHD-C4C-C3C	-2.51	121.17	124.88
16	A3	848	BCR	C1-C6-C5	-2.51	119.06	122.59
14	B2	830	CLA	CHD-C4C-C3C	-2.51	121.18	124.88
14	X2	1701	CLA	CHD-C4C-C3C	-2.51	121.18	124.88
16	A4	849	BCR	C36-C18-C17	-2.51	119.41	122.92
16	B6	847	BCR	C33-C5-C4	-2.51	108.82	113.56
14	B5	1806	CLA	O1D-CGD-CBD	-2.51	119.93	124.58
16	B5	1850	BCR	C33-C5-C4	-2.51	108.82	113.56
16	A2	1648	BCR	C1-C6-C5	-2.51	119.07	122.59
14	B6	835	CLA	CHD-C4C-C3C	-2.50	121.18	124.88
14	B2	825	CLA	CHD-C4C-C3C	-2.50	121.18	124.88
14	A2	1615	CLA	O1D-CGD-CBD	-2.50	119.94	124.58
14	A5	810	CLA	CHD-C4C-C3C	-2.50	121.19	124.88
16	B4	849	BCR	C33-C5-C4	-2.50	108.83	113.56
14	A1	839	CLA	CHD-C4C-C3C	-2.50	121.19	124.88
16	A5	850	BCR	C36-C18-C17	-2.50	119.42	122.92
14	B3	1818	CLA	CHD-C4C-C3C	-2.50	121.19	124.88
14	A6	1602	CLA	CHD-C4C-C3C	-2.50	121.19	124.88
14	B1	834	CLA	CHD-C4C-C3C	-2.50	121.19	124.88
16	B1	844	BCR	C38-C26-C27	-2.50	108.83	113.56
14	B2	818	CLA	CHD-C4C-C3C	-2.50	121.19	124.88
14	B3	1803	CLA	C7-C6-C5	-2.50	106.37	113.17
16	B3	1846	BCR	C38-C26-C27	-2.50	108.83	113.56
14	A5	801	CLA	CHD-C4C-C3C	-2.50	121.19	124.88
14	X3	102	CLA	CHD-C4C-C3C	-2.50	121.19	124.88
14	B3	1804	CLA	OBD-CAD-CBD	-2.50	122.24	125.91
14	A3	818	CLA	CHD-C4C-C3C	-2.50	121.19	124.88
14	B1	803	CLA	O2A-CGA-O1A	-2.50	117.49	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B2	846	BCR	C33-C5-C4	-2.50	108.84	113.56
14	B5	1821	CLA	CHD-C4C-C3C	-2.50	121.20	124.88
14	A2	1629	CLA	CHD-C4C-C3C	-2.49	121.20	124.88
14	B5	1823	CLA	CHD-C4C-C3C	-2.49	121.20	124.88
14	A6	1629	CLA	CHD-C4C-C3C	-2.49	121.20	124.88
14	A4	827	CLA	CHD-C4C-C3C	-2.49	121.20	124.88
14	A3	813	CLA	O1D-CGD-CBD	-2.49	119.95	124.58
14	B5	1802	CLA	CBC-CAC-C3C	-2.49	105.48	112.42
14	B5	1807	CLA	CHD-C4C-C3C	-2.49	121.20	124.88
16	A2	1651	BCR	C23-C22-C21	-2.49	115.12	118.94
14	A4	808	CLA	CHD-C4C-C3C	-2.49	121.20	124.88
14	B1	814	CLA	O1D-CGD-CBD	-2.49	119.96	124.58
16	F6	203	BCR	C1-C6-C5	-2.49	119.09	122.59
16	A6	1643	BCR	C1-C6-C5	-2.49	119.09	122.59
14	B3	1801	CLA	O2A-CGA-O1A	-2.49	117.50	123.58
14	A6	1610	CLA	CHD-C4C-C3C	-2.49	121.21	124.88
14	A5	808	CLA	O1D-CGD-CBD	-2.49	119.96	124.58
14	A1	829	CLA	CHD-C4C-C3C	-2.49	121.21	124.88
16	J5	104	BCR	C1-C6-C5	-2.49	119.09	122.59
14	B2	802	CLA	C1C-C2C-C3C	-2.49	104.27	106.93
14	A3	825	CLA	CHD-C4C-C3C	-2.49	121.21	124.88
16	A1	843	BCR	C1-C6-C5	-2.49	119.10	122.59
14	A4	810	CLA	CHD-C4C-C3C	-2.48	121.21	124.88
14	A3	810	CLA	CHD-C4C-C3C	-2.48	121.21	124.88
16	B2	844	BCR	C1-C6-C5	-2.48	119.10	122.59
14	A4	826	CLA	CHD-C4C-C3C	-2.48	121.22	124.88
14	A4	801	CLA	CBC-CAC-C3C	-2.48	105.51	112.42
16	A4	848	BCR	C23-C22-C21	-2.48	115.13	118.94
16	L1	203	BCR	C19-C18-C17	-2.48	115.13	118.94
14	A2	1602	CLA	CHD-C4C-C3C	-2.48	121.22	124.88
14	X1	1701	CLA	CHD-C4C-C3C	-2.48	121.22	124.88
14	A6	1634	CLA	CHD-C4C-C3C	-2.48	121.22	124.88
14	A6	1619	CLA	O2A-CGA-O1A	-2.48	117.53	123.58
16	A5	849	BCR	C30-C25-C26	-2.48	119.11	122.59
14	A2	1644	CLA	CHD-C4C-C3C	-2.48	121.22	124.88
14	X4	102	CLA	CHD-C4C-C3C	-2.48	121.22	124.88
14	B6	833	CLA	CHD-C4C-C3C	-2.48	121.22	124.88
16	J2	103	BCR	C1-C6-C5	-2.48	119.11	122.59
16	J2	102	BCR	C19-C18-C17	-2.48	115.14	118.94
14	B1	820	CLA	CHD-C4C-C3C	-2.48	121.23	124.88
14	B6	841	CLA	CHD-C4C-C3C	-2.47	121.23	124.88
14	B6	829	CLA	CMB-C2B-C1B	-2.47	124.66	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	817	CLA	O1D-CGD-CBD	-2.47	119.99	124.58
14	X6	1701	CLA	CHD-C4C-C3C	-2.47	121.23	124.88
14	A2	1602	CLA	CBC-CAC-C3C	-2.47	105.54	112.42
14	B4	835	CLA	CHD-C4C-C3C	-2.47	121.23	124.88
14	B5	1815	CLA	O1D-CGD-CBD	-2.47	120.00	124.58
14	L2	207	CLA	CHD-C4C-C3C	-2.47	121.24	124.88
14	A6	1627	CLA	O1D-CGD-CBD	-2.47	120.00	124.58
14	A3	831	CLA	O1D-CGD-CBD	-2.47	120.00	124.58
16	J4	103	BCR	C19-C18-C17	-2.47	115.16	118.94
14	B6	839	CLA	O2A-CGA-O1A	-2.47	117.56	123.58
14	B6	802	CLA	C1C-C2C-C3C	-2.47	104.29	106.93
14	A2	1630	CLA	CHD-C4C-C3C	-2.47	121.24	124.88
14	A1	808	CLA	CHD-C4C-C3C	-2.47	121.24	124.88
14	A3	808	CLA	O1D-CGD-CBD	-2.47	120.01	124.58
14	B5	1822	CLA	O1D-CGD-CBD	-2.47	120.01	124.58
14	A2	1613	CLA	CHD-C4C-C3C	-2.47	121.24	124.88
16	F4	203	BCR	C1-C6-C5	-2.47	119.13	122.59
14	A6	1608	CLA	O2A-CGA-O1A	-2.46	117.57	123.58
16	J4	103	BCR	C30-C25-C26	-2.46	119.13	122.59
16	J1	103	BCR	C19-C18-C17	-2.46	115.16	118.94
14	A4	809	CLA	CHD-C4C-C3C	-2.46	121.25	124.88
14	A5	830	CLA	O1D-CGD-CBD	-2.46	120.02	124.58
16	I4	101	BCR	C19-C18-C17	-2.46	115.17	118.94
14	A6	1627	CLA	CHD-C4C-C3C	-2.46	121.25	124.88
14	B4	804	CLA	OBD-CAD-CBD	-2.46	122.30	125.91
14	A1	817	CLA	O2A-CGA-O1A	-2.46	117.58	123.58
14	B3	1835	CLA	CHD-C4C-C3C	-2.46	121.25	124.88
16	B6	844	BCR	C38-C26-C27	-2.46	108.92	113.56
14	B6	836	CLA	CHD-C4C-C3C	-2.46	121.25	124.88
14	B5	1804	CLA	C1C-C2C-C3C	-2.46	104.30	106.93
16	B1	843	BCR	C1-C6-C5	-2.46	119.14	122.59
14	B2	810	CLA	CHD-C4C-C3C	-2.46	121.26	124.88
16	A1	847	BCR	C36-C18-C17	-2.46	119.48	122.92
16	A5	847	BCR	C1-C6-C5	-2.45	119.14	122.59
14	B1	811	CLA	CHD-C4C-C3C	-2.45	121.26	124.88
14	B4	829	CLA	O1D-CGD-CBD	-2.45	120.03	124.58
14	B5	1818	CLA	CHD-C4C-C3C	-2.45	121.26	124.88
14	A2	1617	CLA	O1D-CGD-CBD	-2.45	120.03	124.58
14	B5	1832	CLA	O1D-CGD-CBD	-2.45	120.03	124.58
14	A1	829	CLA	O1D-CGD-CBD	-2.45	120.03	124.58
14	B6	809	CLA	CHD-C4C-C3C	-2.45	121.26	124.88
14	A6	1603	CLA	CBC-CAC-C3C	-2.45	105.60	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J4	103	BCR	C1-C6-C5	-2.45	119.15	122.59
14	B4	811	CLA	CHD-C4C-C3C	-2.45	121.27	124.88
14	A3	808	CLA	O2A-CGA-O1A	-2.45	117.60	123.58
16	B1	847	BCR	C33-C5-C4	-2.45	108.93	113.56
14	B5	1804	CLA	O1D-CGD-CBD	-2.45	120.04	124.58
14	A5	825	CLA	CHD-C4C-C3C	-2.45	121.27	124.88
14	B3	1841	CLA	CHD-C4C-C3C	-2.45	121.27	124.88
14	L4	205	CLA	CHD-C4C-C3C	-2.45	121.27	124.88
16	B2	844	BCR	C34-C9-C10	-2.45	119.50	122.92
16	B5	1849	BCR	C33-C5-C4	-2.45	108.94	113.56
16	J2	102	BCR	C30-C25-C26	-2.45	119.15	122.59
17	A2	1654	LHG	C6-C5-C4	-2.44	106.34	111.86
14	A1	826	CLA	CHD-C4C-C3C	-2.44	121.27	124.88
14	A4	818	CLA	O2A-CGA-O1A	-2.44	117.62	123.58
14	B1	830	CLA	O2A-CGA-O1A	-2.44	117.62	123.58
14	B4	801	CLA	C1C-C2C-C3C	-2.44	104.32	106.93
14	B2	802	CLA	CHD-C4C-C3C	-2.44	121.28	124.88
14	B2	834	CLA	CHD-C4C-C3C	-2.44	121.28	124.88
16	J1	104	BCR	C1-C6-C5	-2.44	119.16	122.59
14	A6	1634	CLA	O2A-CGA-O1A	-2.44	117.63	123.58
16	A2	1647	BCR	C30-C25-C26	-2.44	119.16	122.59
14	A4	823	CLA	O2A-CGA-O1A	-2.44	117.63	123.58
16	A1	842	BCR	C30-C25-C26	-2.44	119.16	122.59
14	A6	1605	CLA	O1D-CGD-CBD	-2.44	120.06	124.58
14	A3	835	CLA	CHD-C4C-C3C	-2.44	121.28	124.88
14	B3	1823	CLA	CHD-C4C-C3C	-2.44	121.28	124.88
14	B6	823	CLA	CHD-C4C-C3C	-2.44	121.28	124.88
14	A3	830	CLA	O1D-CGD-CBD	-2.44	120.06	124.58
14	B4	802	CLA	CBC-CAC-C3C	-2.44	105.64	112.42
14	B5	1812	CLA	C1C-C2C-C3C	-2.43	104.32	106.93
16	A1	846	BCR	C23-C22-C21	-2.43	115.21	118.94
14	B3	1843	CLA	CHD-C4C-C3C	-2.43	121.29	124.88
16	A5	846	BCR	C1-C6-C5	-2.43	119.17	122.59
14	A4	826	CLA	O2A-CGA-O1A	-2.43	117.64	123.58
14	A2	1624	CLA	CHD-C4C-C3C	-2.43	121.29	124.88
14	B2	832	CLA	CHD-C4C-C3C	-2.43	121.30	124.88
14	B4	825	CLA	CHD-C4C-C3C	-2.43	121.30	124.88
14	B4	837	CLA	CHD-C4C-C3C	-2.43	121.30	124.88
14	L3	202	CLA	CHD-C4C-C3C	-2.43	121.30	124.88
14	A5	827	CLA	CHD-C4C-C3C	-2.43	121.30	124.88
14	M1	1201	CLA	O2A-CGA-O1A	-2.43	117.66	123.58
14	A4	819	CLA	CHD-C4C-C3C	-2.43	121.30	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A5	836	CLA	CHD-C4C-C3C	-2.43	121.30	124.88
14	A3	816	CLA	CHD-C4C-C3C	-2.43	121.30	124.88
14	B4	841	CLA	CHD-C4C-C3C	-2.43	121.30	124.88
16	A3	851	BCR	C30-C25-C26	-2.43	119.18	122.59
14	B5	1842	CLA	CHD-C4C-C3C	-2.42	121.30	124.88
16	A4	846	BCR	C33-C5-C4	-2.42	108.98	113.56
14	A3	802	CLA	C1C-C2C-C3C	-2.42	104.34	106.93
14	B4	826	CLA	CHD-C4C-C3C	-2.42	121.30	124.88
16	A6	1644	BCR	C1-C6-C5	-2.42	119.19	122.59
14	L6	208	CLA	CHD-C4C-C3C	-2.42	121.31	124.88
14	L3	205	CLA	CHD-C4C-C3C	-2.42	121.31	124.88
16	J1	103	BCR	C38-C26-C27	-2.42	108.98	113.56
16	A1	847	BCR	C24-C25-C26	-2.42	115.76	121.54
14	A3	825	CLA	O1D-CGD-CBD	-2.42	120.09	124.58
16	A3	851	BCR	C23-C22-C21	-2.42	115.22	118.94
14	A2	1636	CLA	O2A-CGA-O1A	-2.42	117.67	123.58
16	I3	101	BCR	C19-C18-C17	-2.42	115.23	118.94
14	B2	815	CLA	CHD-C4C-C3C	-2.42	121.31	124.88
16	A5	848	BCR	C30-C25-C26	-2.42	119.19	122.59
14	B1	821	CLA	CHD-C4C-C3C	-2.42	121.31	124.88
14	A5	832	CLA	CHD-C4C-C3C	-2.42	121.31	124.88
14	B2	823	CLA	O1D-CGD-CBD	-2.42	120.10	124.58
14	A5	827	CLA	O1D-CGD-CBD	-2.42	120.10	124.58
14	B4	834	CLA	CHD-C4C-C3C	-2.42	121.31	124.88
16	I6	102	BCR	C19-C18-C17	-2.41	115.24	118.94
14	A3	829	CLA	CHD-C4C-C3C	-2.41	121.32	124.88
14	A6	1609	CLA	CHD-C4C-C3C	-2.41	121.32	124.88
14	B4	809	CLA	O2D-CGD-O1D	-2.41	119.03	123.82
14	B4	803	CLA	C1C-C2C-C3C	-2.41	104.35	106.93
14	A3	820	CLA	CHD-C4C-C3C	-2.41	121.32	124.88
16	J3	104	BCR	C1-C6-C5	-2.41	119.20	122.59
14	A1	818	CLA	O2A-CGA-O1A	-2.41	117.70	123.58
14	B1	822	CLA	O1D-CGD-CBD	-2.41	120.11	124.58
14	B4	815	CLA	CHD-C4C-C3C	-2.41	121.32	124.88
14	A2	1618	CLA	CBC-CAC-C3C	-2.41	105.71	112.42
16	M5	101	BCR	C7-C6-C5	-2.41	115.79	121.54
14	A4	833	CLA	CHD-C4C-C3C	-2.41	121.33	124.88
16	A1	846	BCR	C30-C25-C26	-2.41	119.20	122.59
16	A1	845	BCR	C30-C25-C26	-2.41	119.20	122.59
14	B4	822	CLA	O1D-CGD-CBD	-2.41	120.11	124.58
16	J5	103	BCR	C19-C18-C17	-2.41	115.25	118.94
14	B5	1825	CLA	CHD-C4C-C3C	-2.41	121.33	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	804	CLA	CHD-C4C-C3C	-2.41	121.33	124.88
14	B6	837	CLA	O1D-CGD-CBD	-2.41	120.12	124.58
14	F6	202	CLA	CHD-C4C-C3C	-2.41	121.33	124.88
14	A1	801	CLA	CHD-C4C-C3C	-2.41	121.33	124.88
14	A4	812	CLA	O1D-CGD-CBD	-2.41	120.12	124.58
16	B4	847	BCR	C1-C6-C5	-2.41	119.21	122.59
14	B5	1840	CLA	CBC-CAC-C3C	-2.40	105.73	112.42
14	A6	1627	CLA	O2A-CGA-O1A	-2.40	117.71	123.58
14	A4	831	CLA	CHD-C4C-C3C	-2.40	121.33	124.88
16	B5	1847	BCR	C33-C5-C4	-2.40	109.02	113.56
14	B3	1811	CLA	C12-C11-C10	-2.40	101.83	113.23
16	A3	852	BCR	C36-C18-C17	-2.40	119.56	122.92
14	A2	1618	CLA	CHD-C4C-C3C	-2.40	121.33	124.88
14	A2	1629	CLA	O1D-CGD-CBD	-2.40	120.12	124.58
16	J3	103	BCR	C30-C25-C26	-2.40	119.22	122.59
16	B2	843	BCR	C38-C26-C27	-2.40	109.02	113.56
14	B1	815	CLA	CHD-C4C-C3C	-2.40	121.34	124.88
16	A6	1648	BCR	C36-C18-C17	-2.40	119.56	122.92
16	J3	103	BCR	C19-C18-C17	-2.40	115.26	118.94
14	A1	839	CLA	C1C-C2C-C3C	-2.40	104.36	106.93
14	A5	819	CLA	O2A-CGA-O1A	-2.40	117.73	123.58
16	J6	1104	BCR	C30-C25-C26	-2.40	119.22	122.59
16	F2	203	BCR	C1-C6-C5	-2.40	119.22	122.59
14	A2	1610	CLA	O2A-CGA-O1A	-2.39	117.74	123.58
14	A3	845	CLA	O2A-CGA-O1A	-2.39	117.74	123.58
16	A3	850	BCR	C30-C25-C26	-2.39	119.23	122.59
14	B4	807	CLA	OBD-CAD-CBD	-2.39	122.39	125.91
14	B4	801	CLA	OBD-CAD-CBD	-2.39	122.39	125.91
16	I5	101	BCR	C19-C18-C17	-2.39	115.27	118.94
14	B5	1841	CLA	CHD-C4C-C3C	-2.39	121.35	124.88
14	A2	1611	CLA	O2A-CGA-O1A	-2.39	117.74	123.58
14	B5	1816	CLA	CHD-C4C-C3C	-2.39	121.35	124.88
14	F2	204	CLA	CAA-C2A-C3A	-2.39	110.42	116.06
14	A6	1601	CLA	O2D-CGD-O1D	-2.39	119.07	123.82
16	A6	1647	BCR	C30-C25-C26	-2.39	119.23	122.59
14	A1	807	CLA	O1D-CGD-CBD	-2.39	120.14	124.58
14	B6	814	CLA	CHD-C4C-C3C	-2.39	121.35	124.88
16	A5	850	BCR	C24-C25-C26	-2.39	115.84	121.54
14	B3	1823	CLA	O1D-CGD-CBD	-2.39	120.15	124.58
14	B1	833	CLA	O1D-CGD-CBD	-2.39	120.15	124.58
16	A4	847	BCR	C30-C25-C26	-2.39	119.23	122.59
14	X5	101	CLA	CHD-C4C-C3C	-2.39	121.35	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B2	802	CLA	O2A-CGA-O1A	-2.39	117.75	123.58
14	L1	207	CLA	CHD-C4C-C3C	-2.39	121.36	124.88
14	A5	822	CLA	CHD-C4C-C3C	-2.39	121.36	124.88
16	J6	1104	BCR	C19-C18-C17	-2.39	115.28	118.94
14	B6	832	CLA	CHD-C4C-C3C	-2.38	121.36	124.88
14	B3	1821	CLA	CHD-C4C-C3C	-2.38	121.36	124.88
14	A1	832	CLA	CHD-C4C-C3C	-2.38	121.36	124.88
14	A2	1604	CLA	CBC-CAC-C3C	-2.38	105.79	112.42
16	B6	850	BCR	C33-C5-C4	-2.38	109.06	113.56
14	B1	822	CLA	CHD-C4C-C3C	-2.38	121.36	124.88
16	A1	842	BCR	C1-C6-C5	-2.38	119.24	122.59
14	B6	802	CLA	CBC-CAC-C3C	-2.38	105.79	112.42
14	A2	1629	CLA	O2A-CGA-O1A	-2.38	117.77	123.58
14	B5	1804	CLA	OBD-CAD-CBD	-2.38	122.41	125.91
14	A3	801	CLA	CBC-CAC-C3C	-2.38	105.79	112.42
16	B1	845	BCR	C1-C6-C5	-2.38	119.24	122.59
14	B4	803	CLA	CHD-C4C-C3C	-2.38	121.37	124.88
14	B6	819	CLA	CHD-C4C-C3C	-2.38	121.37	124.88
16	M3	1602	BCR	C7-C6-C5	-2.38	115.87	121.54
16	J3	103	BCR	C38-C26-C27	-2.38	109.06	113.56
14	B2	801	CLA	CHD-C4C-C3C	-2.38	121.37	124.88
14	L1	201	CLA	CHD-C4C-C3C	-2.38	121.37	124.88
14	A6	1620	CLA	CHD-C4C-C3C	-2.38	121.37	124.88
16	A3	849	BCR	C33-C5-C4	-2.38	109.07	113.56
16	A2	1649	BCR	C33-C5-C4	-2.38	109.07	113.56
14	B4	838	CLA	CHD-C4C-C3C	-2.38	121.38	124.88
16	B2	844	BCR	C33-C5-C4	-2.37	109.07	113.56
14	B1	839	CLA	CBC-CAC-C3C	-2.37	105.81	112.42
14	B5	1835	CLA	CHD-C4C-C3C	-2.37	121.38	124.88
14	A5	815	CLA	O1D-CGD-CBD	-2.37	120.18	124.58
14	A4	841	CLA	CHD-C4C-C3C	-2.37	121.38	124.88
14	A6	1625	CLA	CHD-C4C-C3C	-2.37	121.38	124.88
14	B4	823	CLA	O1D-CGD-CBD	-2.37	120.18	124.58
14	A1	823	CLA	O2A-CGA-O1A	-2.37	117.79	123.58
14	B1	811	CLA	C1C-C2C-C3C	-2.37	104.39	106.93
16	A6	1647	BCR	C23-C22-C21	-2.37	115.30	118.94
14	B1	823	CLA	OBD-CAD-CBD	-2.37	122.43	125.91
14	A1	819	CLA	CHD-C4C-C3C	-2.37	121.38	124.88
14	A2	1624	CLA	O1D-CGD-CBD	-2.37	120.18	124.58
14	A4	833	CLA	O2A-CGA-O1A	-2.37	117.80	123.58
14	A6	1616	CLA	CHD-C4C-C3C	-2.37	121.38	124.88
16	L2	208	BCR	C24-C25-C26	-2.37	115.89	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	839	CLA	CHD-C4C-C3C	-2.37	121.38	124.88
16	A2	1650	BCR	C30-C25-C26	-2.37	119.26	122.59
14	A2	1606	CLA	CHD-C4C-C3C	-2.37	121.39	124.88
16	A6	1646	BCR	C30-C25-C26	-2.37	119.26	122.59
16	L6	209	BCR	C24-C25-C26	-2.37	115.89	121.54
14	A1	803	CLA	CHD-C4C-C3C	-2.37	121.39	124.88
14	A4	815	CLA	CBC-CAC-C3C	-2.37	105.83	112.42
14	A3	806	CLA	O2A-CGA-O1A	-2.37	117.81	123.58
14	J6	1103	CLA	CAA-C2A-C3A	-2.37	110.48	116.06
14	A6	1602	CLA	CBC-CAC-C3C	-2.37	105.84	112.42
16	J1	103	BCR	C30-C25-C26	-2.37	119.27	122.59
14	A3	835	CLA	O2A-CGA-O1A	-2.36	117.81	123.58
14	A4	853	CLA	CHD-C4C-C3C	-2.36	121.39	124.88
14	B2	820	CLA	CHD-C4C-C3C	-2.36	121.39	124.88
14	A3	819	CLA	O2A-CGA-O1A	-2.36	117.81	123.58
14	B3	1803	CLA	C1C-C2C-C3C	-2.36	104.40	106.93
14	A4	853	CLA	O2D-CGD-O1D	-2.36	119.13	123.82
14	A2	1620	CLA	O2A-CGA-O1A	-2.36	117.81	123.58
16	B2	842	BCR	C33-C5-C4	-2.36	109.10	113.56
14	A1	824	CLA	O1D-CGD-CBD	-2.36	120.20	124.58
14	A5	827	CLA	O2A-CGA-O1A	-2.36	117.82	123.58
14	B5	1834	CLA	CHD-C4C-C3C	-2.36	121.40	124.88
14	B4	832	CLA	O1D-CGD-CBD	-2.36	120.20	124.58
16	B6	843	BCR	C33-C5-C4	-2.36	109.10	113.56
14	B2	823	CLA	CHD-C4C-C3C	-2.36	121.40	124.88
14	A4	817	CLA	O2A-CGA-O1A	-2.36	117.82	123.58
16	L4	206	BCR	C24-C25-C26	-2.36	115.91	121.54
14	B3	1840	CLA	CBC-CAC-C3C	-2.36	105.85	112.42
16	A6	1645	BCR	C33-C5-C4	-2.36	109.10	113.56
14	B2	822	CLA	CHD-C4C-C3C	-2.36	121.40	124.88
16	M4	101	BCR	C33-C5-C4	-2.36	109.11	113.56
14	A6	1651	CLA	C1C-C2C-C3C	-2.36	104.41	106.93
14	K5	102	CLA	CHD-C4C-C3C	-2.36	121.40	124.88
16	F3	203	BCR	C33-C5-C4	-2.36	109.11	113.56
14	A3	818	CLA	O2A-CGA-O1A	-2.36	117.83	123.58
14	A5	834	CLA	O2A-CGA-O1A	-2.36	117.83	123.58
14	B1	801	CLA	C1C-C2C-C3C	-2.36	104.41	106.93
16	B2	845	BCR	C19-C18-C17	-2.36	115.33	118.94
14	A1	812	CLA	O1D-CGD-CBD	-2.36	120.21	124.58
14	B5	1837	CLA	CHD-C4C-C3C	-2.36	121.40	124.88
14	B1	824	CLA	CHD-C4C-C3C	-2.36	121.40	124.88
14	B2	802	CLA	OBD-CAD-CBD	-2.36	122.45	125.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B3	1806	CLA	O2A-CGA-O1A	-2.35	117.83	123.58
14	B2	826	CLA	O1D-CGD-CBD	-2.35	120.21	124.58
14	A1	820	CLA	C12-C11-C10	-2.35	102.06	113.23
16	J4	103	BCR	C12-C13-C14	-2.35	115.33	118.94
14	B5	1831	CLA	O2A-CGA-O1A	-2.35	117.84	123.58
14	J3	102	CLA	CAA-C2A-C3A	-2.35	110.51	116.06
14	A3	827	CLA	O2A-CGA-O1A	-2.35	117.84	123.58
14	B1	804	CLA	C1C-C2C-C3C	-2.35	104.41	106.93
14	L6	202	CLA	CHD-C4C-C3C	-2.35	121.41	124.88
14	B3	1819	CLA	CHD-C4C-C3C	-2.35	121.41	124.88
14	A5	822	CLA	O1D-CGD-CBD	-2.35	120.22	124.58
14	J4	102	CLA	CAA-C2A-C3A	-2.35	110.51	116.06
14	B2	831	CLA	CHD-C4C-C3C	-2.35	121.41	124.88
14	A1	827	CLA	O2A-CGA-O1A	-2.35	117.84	123.58
16	A4	848	BCR	C30-C25-C26	-2.35	119.29	122.59
16	A1	844	BCR	C33-C5-C4	-2.35	109.12	113.56
14	A2	1621	CLA	O2A-CGA-O1A	-2.35	117.84	123.58
14	A3	804	CLA	CHD-C4C-C3C	-2.35	121.41	124.88
16	B4	849	BCR	C19-C18-C17	-2.35	115.34	118.94
14	L2	206	CLA	CHD-C4C-C3C	-2.35	121.41	124.88
14	B3	1803	CLA	CHD-C4C-C3C	-2.35	121.42	124.88
16	B3	1845	BCR	C33-C5-C4	-2.35	109.13	113.56
14	B5	1839	CLA	O1D-CGD-CBD	-2.35	120.23	124.58
14	B2	817	CLA	O2A-CGA-O1A	-2.35	117.86	123.58
16	A4	849	BCR	C24-C25-C26	-2.35	115.95	121.54
14	A3	802	CLA	O2D-CGD-O1D	-2.34	119.17	123.82
16	B5	1847	BCR	C1-C6-C5	-2.34	119.30	122.59
14	A1	821	CLA	CHD-C4C-C3C	-2.34	121.42	124.88
16	L5	207	BCR	C24-C25-C26	-2.34	115.95	121.54
16	M2	1202	BCR	C33-C5-C4	-2.34	109.13	113.56
16	F3	203	BCR	C1-C6-C5	-2.34	119.30	122.59
14	L2	205	CLA	O2A-CGA-O1A	-2.34	117.86	123.58
14	A5	833	CLA	CHD-C4C-C3C	-2.34	121.42	124.88
14	B1	825	CLA	O1D-CGD-CBD	-2.34	120.24	124.58
14	J1	102	CLA	CAA-C2A-C3A	-2.34	110.53	116.06
14	B4	823	CLA	CHD-C4C-C3C	-2.34	121.42	124.88
14	A1	815	CLA	CBC-CAC-C3C	-2.34	105.90	112.42
14	A4	821	CLA	O1D-CGD-CBD	-2.34	120.24	124.58
14	B2	836	CLA	O1D-CGD-CBD	-2.34	120.24	124.58
16	A6	1648	BCR	C24-C25-C26	-2.34	115.96	121.54
14	A6	1613	CLA	O1D-CGD-CBD	-2.34	120.24	124.58
16	J6	1104	BCR	C12-C13-C14	-2.34	115.35	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I2	101	BCR	C19-C18-C17	-2.34	115.35	118.94
16	A5	847	BCR	C33-C5-C4	-2.34	109.14	113.56
14	A3	802	CLA	CBC-CAC-C3C	-2.34	105.91	112.42
14	B6	837	CLA	O2A-CGA-O1A	-2.34	117.88	123.58
14	K1	1401	CLA	CHD-C4C-C3C	-2.34	121.43	124.88
14	K4	1401	CLA	CHD-C4C-C3C	-2.34	121.43	124.88
14	K2	1401	CLA	CHD-C4C-C3C	-2.34	121.43	124.88
14	A1	837	CLA	O2A-CGA-O1A	-2.34	117.88	123.58
14	A6	1604	CLA	CHD-C4C-C3C	-2.34	121.43	124.88
16	A2	1651	BCR	C30-C25-C26	-2.34	119.31	122.59
14	A3	822	CLA	O1D-CGD-CBD	-2.33	120.25	124.58
14	L1	206	CLA	CHD-C4C-C3C	-2.33	121.44	124.88
14	A2	1601	CLA	CHD-C4C-C3C	-2.33	121.44	124.88
14	B6	821	CLA	O1D-CGD-CBD	-2.33	120.25	124.58
14	B1	853	CLA	O2A-CGA-O1A	-2.33	117.89	123.58
14	J5	102	CLA	CAA-C2A-C3A	-2.33	110.56	116.06
14	B1	805	CLA	CHD-C4C-C3C	-2.33	121.44	124.88
14	L5	205	CLA	CHD-C4C-C3C	-2.33	121.44	124.88
14	A5	802	CLA	C1C-C2C-C3C	-2.33	104.44	106.93
14	A1	801	CLA	CBC-CAC-C3C	-2.33	105.93	112.42
14	B4	852	CLA	O2A-CGA-O1A	-2.33	117.89	123.58
14	A6	1638	CLA	CHD-C4C-C3C	-2.33	121.44	124.88
14	A5	843	CLA	O2A-CGA-O1A	-2.33	117.89	123.58
16	F6	203	BCR	C33-C5-C4	-2.33	109.16	113.56
14	B4	811	CLA	C12-C11-C10	-2.33	102.17	113.23
16	B4	847	BCR	C33-C5-C4	-2.33	109.16	113.56
16	B1	845	BCR	C33-C5-C4	-2.33	109.16	113.56
14	F3	202	CLA	CHD-C4C-C3C	-2.33	121.44	124.88
14	B1	833	CLA	CHD-C4C-C3C	-2.33	121.45	124.88
14	A3	809	CLA	CHD-C4C-C3C	-2.33	121.45	124.88
14	B2	808	CLA	C12-C11-C10	-2.33	102.19	113.23
14	B2	826	CLA	O2A-CGA-O1A	-2.33	117.90	123.58
14	B4	840	CLA	CBC-CAC-C3C	-2.33	105.95	112.42
14	A5	824	CLA	O2A-CGA-O1A	-2.33	117.91	123.58
14	B4	818	CLA	CHD-C4C-C3C	-2.33	121.45	124.88
14	L5	206	CLA	CHD-C4C-C3C	-2.32	121.45	124.88
14	B1	804	CLA	CHD-C4C-C3C	-2.32	121.45	124.88
14	A5	804	CLA	CHD-C4C-C3C	-2.32	121.45	124.88
14	A6	1622	CLA	CHD-C4C-C3C	-2.32	121.45	124.88
16	B3	1847	BCR	C33-C5-C4	-2.32	109.17	113.56
16	A5	850	BCR	C33-C5-C4	-2.32	109.17	113.56
14	B3	1834	CLA	CHD-C4C-C3C	-2.32	121.45	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A5	831	CLA	O2A-CGA-O1A	-2.32	117.91	123.58
14	A4	826	CLA	O1D-CGD-CBD	-2.32	120.27	124.58
14	B1	811	CLA	C12-C11-C10	-2.32	102.22	113.23
14	A5	809	CLA	CHD-C4C-C3C	-2.32	121.45	124.88
14	A6	1639	CLA	O2A-CGA-O1A	-2.32	117.92	123.58
14	B6	805	CLA	C12-C11-C10	-2.32	102.22	113.23
16	B6	845	BCR	C33-C5-C4	-2.32	109.18	113.56
14	B3	1804	CLA	C1C-C2C-C3C	-2.32	104.45	106.93
16	J4	104	BCR	C1-C6-C5	-2.32	119.33	122.59
14	A1	807	CLA	O2A-CGA-O1A	-2.32	117.92	123.58
14	A2	1623	CLA	C12-C11-C10	-2.32	102.23	113.23
14	B3	1820	CLA	O2A-CGA-O1A	-2.32	117.92	123.58
16	J2	102	BCR	C38-C26-C27	-2.32	109.18	113.56
16	A5	849	BCR	C23-C22-C21	-2.32	115.39	118.94
14	B4	801	CLA	O2D-CGD-O1D	-2.32	119.22	123.82
14	A2	1603	CLA	C1C-C2C-C3C	-2.32	104.45	106.93
16	A3	849	BCR	C1-C6-C5	-2.32	119.34	122.59
16	B4	847	BCR	C34-C9-C10	-2.32	119.68	122.92
14	A5	834	CLA	CHD-C4C-C3C	-2.31	121.47	124.88
14	B2	801	CLA	C1C-C2C-C3C	-2.31	104.45	106.93
14	B1	828	CLA	C1C-C2C-C3C	-2.31	104.45	106.93
14	B2	837	CLA	CBC-CAC-C3C	-2.31	105.98	112.42
14	B3	1842	CLA	CHD-C4C-C3C	-2.31	121.47	124.88
14	B6	818	CLA	O2A-CGA-O1A	-2.31	117.94	123.58
14	B6	821	CLA	CHD-C4C-C3C	-2.31	121.47	124.88
14	B1	837	CLA	CHD-C4C-C3C	-2.31	121.47	124.88
15	B3	1844	PQN	C17-C16-C15	-2.31	106.88	113.17
14	B2	815	CLA	O2A-CGA-O1A	-2.31	117.94	123.58
14	A4	815	CLA	CHD-C4C-C3C	-2.31	121.47	124.88
14	A1	836	CLA	CHD-C4C-C3C	-2.31	121.47	124.88
14	A4	839	CLA	O2A-CGA-O1A	-2.31	117.94	123.58
16	F5	1302	BCR	C1-C6-C5	-2.31	119.34	122.59
14	A4	819	CLA	O2A-CGA-O1A	-2.31	117.94	123.58
14	A4	821	CLA	CHD-C4C-C3C	-2.31	121.47	124.88
14	B5	1840	CLA	CHD-C4C-C3C	-2.31	121.47	124.88
14	A2	1601	CLA	O2D-CGD-O1D	-2.31	119.24	123.82
14	A4	813	CLA	O1D-CGD-CBD	-2.31	120.30	124.58
16	J5	103	BCR	C38-C26-C27	-2.31	109.20	113.56
14	A5	814	CLA	O1D-CGD-CBD	-2.31	120.30	124.58
14	B2	817	CLA	CHD-C4C-C3C	-2.31	121.47	124.88
14	B3	1804	CLA	O2A-CGA-O1A	-2.31	117.95	123.58
14	A2	1617	CLA	CHD-C4C-C3C	-2.31	121.47	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	810	CLA	CHD-C4C-C3C	-2.31	121.47	124.88
14	B4	826	CLA	O1D-CGD-CBD	-2.31	120.30	124.58
16	B3	1849	BCR	C19-C18-C17	-2.31	115.40	118.94
14	B6	824	CLA	O1D-CGD-CBD	-2.31	120.30	124.58
14	J3	102	CLA	CHD-C4C-C3C	-2.31	121.48	124.88
14	B2	813	CLA	CHD-C4C-C3C	-2.31	121.48	124.88
14	K6	1401	CLA	CHD-C4C-C3C	-2.31	121.48	124.88
14	A6	1618	CLA	O2A-CGA-O1A	-2.31	117.95	123.58
14	A2	1636	CLA	CHD-C4C-C3C	-2.31	121.48	124.88
14	B5	1842	CLA	C4C-C3C-C2C	-2.31	103.48	106.90
14	B5	1831	CLA	C1C-C2C-C3C	-2.31	104.46	106.93
14	A1	821	CLA	O1D-CGD-CBD	-2.31	120.30	124.58
14	F4	202	CLA	CHD-C4C-C3C	-2.30	121.48	124.88
14	A5	808	CLA	O2A-CGA-O1A	-2.30	117.96	123.58
14	B3	1828	CLA	CMB-C2B-C1B	-2.30	124.92	128.46
14	B5	1838	CLA	CHD-C4C-C3C	-2.30	121.48	124.88
14	B6	840	CLA	CHD-C4C-C3C	-2.30	121.48	124.88
14	B3	1811	CLA	C1C-C2C-C3C	-2.30	104.47	106.93
14	B5	1826	CLA	CHD-C4C-C3C	-2.30	121.48	124.88
14	B4	811	CLA	C1C-C2C-C3C	-2.30	104.47	106.93
16	I4	102	BCR	C38-C26-C27	-2.30	109.21	113.56
14	B4	839	CLA	O1D-CGD-CBD	-2.30	120.31	124.58
16	F1	1302	BCR	C33-C5-C4	-2.30	109.21	113.56
14	B4	806	CLA	O2A-CGA-O1A	-2.30	117.96	123.58
14	A2	1626	CLA	O2A-CGA-O1A	-2.30	117.97	123.58
16	F2	203	BCR	C33-C5-C4	-2.30	109.21	113.56
14	B1	854	CLA	CHD-C4C-C3C	-2.30	121.49	124.88
14	B6	827	CLA	O1D-CGD-CBD	-2.30	120.31	124.58
16	L2	203	BCR	C38-C26-C27	-2.30	109.22	113.56
16	A4	844	BCR	C30-C25-C26	-2.30	119.36	122.59
14	L4	204	CLA	CHD-C4C-C3C	-2.30	121.49	124.88
16	J2	102	BCR	C12-C13-C14	-2.30	115.42	118.94
16	L1	209	BCR	C1-C6-C5	-2.30	119.36	122.59
16	B6	845	BCR	C30-C25-C26	-2.30	119.36	122.59
14	A3	808	CLA	CBC-CAC-C3C	-2.30	106.03	112.42
16	A3	852	BCR	C33-C5-C4	-2.30	109.22	113.56
14	A5	813	CLA	O1D-CGD-CBD	-2.30	120.32	124.58
16	I3	102	BCR	C30-C25-C26	-2.30	119.36	122.59
14	B5	1820	CLA	O2A-CGA-O1A	-2.30	117.98	123.58
14	A4	814	CLA	O1D-CGD-CBD	-2.30	120.32	124.58
16	M1	1202	BCR	C7-C6-C5	-2.30	116.07	121.54
14	B6	834	CLA	CHD-C4C-C3C	-2.30	121.49	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I5	101	BCR	C1-C6-C5	-2.29	119.37	122.59
16	B4	845	BCR	C33-C5-C4	-2.29	109.22	113.56
16	J6	1105	BCR	C1-C6-C5	-2.29	119.37	122.59
14	A2	1616	CLA	O1D-CGD-CBD	-2.29	120.33	124.58
14	B3	1815	CLA	CHD-C4C-C3C	-2.29	121.50	124.88
14	B1	829	CLA	CHD-C4C-C3C	-2.29	121.50	124.88
14	B6	838	CLA	CBC-CAC-C3C	-2.29	106.04	112.42
14	L4	203	CLA	O2A-CGA-O1A	-2.29	117.98	123.58
14	A1	832	CLA	O2A-CGA-O1A	-2.29	117.99	123.58
14	B6	829	CLA	C1C-C2C-C3C	-2.29	104.48	106.93
14	A4	801	CLA	C1C-C2C-C3C	-2.29	104.48	106.93
14	B2	819	CLA	O1D-CGD-CBD	-2.29	120.33	124.58
14	I1	101	CLA	CHD-C4C-C3C	-2.29	121.50	124.88
14	F5	1301	CLA	CHD-C4C-C3C	-2.29	121.50	124.88
14	B6	809	CLA	C12-C11-C10	-2.29	102.37	113.23
14	B6	804	CLA	C7-C6-C5	-2.29	106.94	113.17
14	B3	1841	CLA	O2A-CGA-O1A	-2.29	118.00	123.58
14	A2	1642	CLA	O2A-CGA-O1A	-2.29	118.00	123.58
14	B3	1840	CLA	CHD-C4C-C3C	-2.29	121.51	124.88
14	B3	1812	CLA	CHD-C4C-C3C	-2.29	121.51	124.88
16	I1	103	BCR	C24-C25-C26	-2.29	116.09	121.54
14	B2	806	CLA	O2D-CGD-O1D	-2.28	119.29	123.82
14	A4	820	CLA	C12-C11-C10	-2.28	102.39	113.23
16	L5	201	BCR	C1-C6-C5	-2.28	119.38	122.59
14	L6	207	CLA	CHD-C4C-C3C	-2.28	121.51	124.88
14	B4	818	CLA	O2A-CGA-O1A	-2.28	118.01	123.58
14	B6	826	CLA	O1D-CGD-CBD	-2.28	120.34	124.58
14	A3	832	CLA	CHD-C4C-C3C	-2.28	121.51	124.88
14	A2	1638	CLA	O1D-CGD-CBD	-2.28	120.35	124.58
14	B1	830	CLA	C1C-C2C-C3C	-2.28	104.49	106.93
16	J3	103	BCR	C12-C13-C14	-2.28	115.44	118.94
14	A3	821	CLA	C12-C11-C10	-2.28	102.41	113.23
14	B1	831	CLA	O1D-CGD-CBD	-2.28	120.35	124.58
14	F1	1301	CLA	CHD-C4C-C3C	-2.28	121.52	124.88
14	A2	1634	CLA	CHD-C4C-C3C	-2.28	121.52	124.88
14	B6	809	CLA	C1C-C2C-C3C	-2.28	104.49	106.93
14	B3	1809	CLA	O2D-CGD-O1D	-2.28	119.30	123.82
14	B2	828	CLA	C1C-C2C-C3C	-2.28	104.49	106.93
16	A6	1648	BCR	C33-C5-C4	-2.28	109.25	113.56
16	J1	103	BCR	C12-C13-C14	-2.28	115.44	118.94
14	B6	818	CLA	CHD-C4C-C3C	-2.28	121.52	124.88
14	A1	830	CLA	CHD-C4C-C3C	-2.28	121.52	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A2	1635	CLA	CHD-C4C-C3C	-2.28	121.52	124.88
14	A2	1606	CLA	C12-C11-C10	-2.28	105.62	113.59
14	B3	1818	CLA	O2A-CGA-O1A	-2.28	118.02	123.58
14	A6	1615	CLA	O1D-CGD-CBD	-2.28	120.36	124.58
14	A3	803	CLA	CHD-C4C-C3C	-2.28	121.52	124.88
14	A6	1616	CLA	CBC-CAC-C3C	-2.28	106.08	112.42
14	A5	805	CLA	O1D-CGD-CBD	-2.28	120.36	124.58
14	B3	1832	CLA	O1D-CGD-CBD	-2.28	120.36	124.58
14	I1	101	CLA	C4C-C3C-C2C	-2.28	103.53	106.90
14	B3	1829	CLA	O2A-CGA-O1A	-2.28	118.03	123.58
16	B6	847	BCR	C19-C18-C17	-2.27	115.45	118.94
14	B5	1822	CLA	CHD-C4C-C3C	-2.27	121.52	124.88
14	A1	838	CLA	C4C-C3C-C2C	-2.27	103.53	106.90
16	A2	1649	BCR	C30-C25-C26	-2.27	119.39	122.59
14	A4	814	CLA	CHD-C4C-C3C	-2.27	121.53	124.88
14	A4	840	CLA	C4C-C3C-C2C	-2.27	103.53	106.90
14	A6	1621	CLA	C12-C11-C10	-2.27	102.45	113.23
16	B3	1847	BCR	C30-C25-C26	-2.27	119.40	122.59
14	A2	1627	CLA	O1D-CGD-CBD	-2.27	120.37	124.58
16	M6	1202	BCR	C33-C5-C4	-2.27	109.27	113.56
14	A3	815	CLA	CHD-C4C-C3C	-2.27	121.53	124.88
14	B6	838	CLA	CHD-C4C-C3C	-2.27	121.53	124.88
14	B2	839	CLA	CHD-C4C-C3C	-2.27	121.53	124.88
14	B2	827	CLA	CHD-C4C-C3C	-2.27	121.53	124.88
14	A6	1651	CLA	O1D-CGD-CBD	-2.27	120.37	124.58
14	B4	842	CLA	CHD-C4C-C3C	-2.27	121.53	124.88
14	A3	822	CLA	CHD-C4C-C3C	-2.27	121.53	124.88
16	A3	847	BCR	C38-C26-C27	-2.27	109.28	113.56
14	A6	1628	CLA	O2A-CGA-O1A	-2.27	118.05	123.58
14	B2	838	CLA	O2A-CGA-O1A	-2.27	118.05	123.58
16	L3	206	BCR	C38-C26-C27	-2.27	109.28	113.56
14	A1	826	CLA	O2A-CGA-O1A	-2.27	118.05	123.58
14	B5	1811	CLA	C12-C11-C10	-2.27	102.48	113.23
14	A1	803	CLA	O2A-CGA-O1A	-2.27	118.05	123.58
14	A2	1630	CLA	O2A-CGA-O1A	-2.27	118.05	123.58
14	B6	804	CLA	C1C-C2C-C3C	-2.27	104.50	106.93
14	A6	1624	CLA	O2A-CGA-O1A	-2.27	118.05	123.58
16	L3	201	BCR	C1-C6-C5	-2.27	119.41	122.59
14	A3	816	CLA	CBC-CAC-C3C	-2.27	106.11	112.42
14	A6	1614	CLA	O1D-CGD-CBD	-2.26	120.38	124.58
16	J2	102	BCR	C1-C6-C5	-2.26	119.41	122.59
16	A3	848	BCR	C30-C25-C26	-2.26	119.41	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M2	1201	CLA	O1D-CGD-CBD	-2.26	120.38	124.58
14	B5	1829	CLA	O1D-CGD-CBD	-2.26	120.38	124.58
14	A1	831	CLA	CHD-C4C-C3C	-2.26	121.54	124.88
14	A1	830	CLA	O2A-CGA-O1A	-2.26	118.06	123.58
14	A5	801	CLA	CBC-CAC-C3C	-2.26	106.13	112.42
14	A5	842	CLA	C1C-C2C-C3C	-2.26	104.51	106.93
14	B5	1803	CLA	C1C-C2C-C3C	-2.26	104.51	106.93
14	B4	816	CLA	CHD-C4C-C3C	-2.26	121.54	124.88
16	M6	1202	BCR	C7-C6-C5	-2.26	116.15	121.54
16	L6	204	BCR	C38-C26-C27	-2.26	109.29	113.56
16	I3	102	BCR	C38-C26-C27	-2.26	109.29	113.56
14	A3	814	CLA	CHD-C4C-C3C	-2.26	121.55	124.88
14	A2	1603	CLA	O2D-CGD-O1D	-2.26	119.34	123.82
16	F1	1302	BCR	C1-C6-C5	-2.26	119.42	122.59
16	F5	1302	BCR	C33-C5-C4	-2.26	109.29	113.56
14	B1	805	CLA	O1D-CGD-CBD	-2.26	120.39	124.58
14	B6	804	CLA	CHD-C4C-C3C	-2.26	121.55	124.88
14	A6	1651	CLA	O2A-CGA-O1A	-2.26	118.07	123.58
14	B1	836	CLA	CHD-C4C-C3C	-2.26	121.55	124.88
14	B5	1819	CLA	CHD-C4C-C3C	-2.26	121.55	124.88
16	I6	102	BCR	C1-C6-C5	-2.26	119.42	122.59
16	A4	845	BCR	C30-C25-C26	-2.26	119.42	122.59
16	J6	1104	BCR	C38-C26-C27	-2.26	109.30	113.56
14	B1	838	CLA	O1D-CGD-CBD	-2.26	120.40	124.58
16	B5	1848	BCR	C19-C18-C17	-2.26	115.48	118.94
14	A4	803	CLA	CHD-C4C-C3C	-2.26	121.55	124.88
14	B5	1806	CLA	O2A-CGA-O1A	-2.26	118.08	123.58
16	L3	201	BCR	C33-C5-C4	-2.26	109.30	113.56
14	B5	1834	CLA	C12-C11-C10	-2.26	102.53	113.23
14	B1	828	CLA	O2A-CGA-O1A	-2.25	118.08	123.58
14	A3	834	CLA	O2D-CGD-O1D	-2.25	119.35	123.82
14	B6	802	CLA	O2D-CGD-O1D	-2.25	119.35	123.82
14	A2	1643	CLA	C4C-C3C-C2C	-2.25	103.56	106.90
15	B1	842	PQN	C17-C16-C15	-2.25	107.04	113.17
14	L3	204	CLA	CHD-C4C-C3C	-2.25	121.56	124.88
14	A5	815	CLA	CHD-C4C-C3C	-2.25	121.56	124.88
14	A5	803	CLA	O1D-CGD-CBD	-2.25	120.40	124.58
14	A3	831	CLA	CHD-C4C-C3C	-2.25	121.56	124.88
14	A3	841	CLA	O1D-CGD-CBD	-2.25	120.41	124.58
16	A2	1652	BCR	C24-C25-C26	-2.25	116.17	121.54
16	L1	209	BCR	C30-C25-C26	-2.25	119.43	122.59
14	B3	1816	CLA	CHD-C4C-C3C	-2.25	121.56	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B2	809	CLA	CHD-C4C-C3C	-2.25	121.56	124.88
16	A4	844	BCR	C38-C26-C27	-2.25	109.31	113.56
16	L1	203	BCR	C38-C26-C27	-2.25	109.31	113.56
14	A1	814	CLA	CHD-C4C-C3C	-2.25	121.56	124.88
14	B2	819	CLA	CHD-C4C-C3C	-2.25	121.56	124.88
16	A2	1647	BCR	C38-C26-C27	-2.25	109.31	113.56
14	A6	1609	CLA	O2A-CGA-O1A	-2.25	118.09	123.58
14	B5	1841	CLA	O2A-CGA-O1A	-2.25	118.09	123.58
16	A3	852	BCR	C24-C25-C26	-2.25	116.18	121.54
14	L3	204	CLA	O2A-CGA-O1A	-2.25	118.09	123.58
16	B4	849	BCR	C30-C25-C26	-2.25	119.43	122.59
14	A1	813	CLA	CHD-C4C-C3C	-2.25	121.56	124.88
14	A4	841	CLA	C1C-C2C-C3C	-2.25	104.53	106.93
14	A4	804	CLA	O1D-CGD-CBD	-2.25	120.41	124.58
14	M3	1601	CLA	O2D-CGD-O1D	-2.25	119.36	123.82
14	A4	832	CLA	CHD-C4C-C3C	-2.25	121.57	124.88
14	B3	1831	CLA	O2A-CGA-O1A	-2.25	118.10	123.58
14	A5	809	CLA	O2A-CGA-O1A	-2.24	118.10	123.58
14	B1	825	CLA	CHD-C4C-C3C	-2.24	121.57	124.88
14	A3	839	CLA	CHD-C4C-C3C	-2.24	121.57	124.88
16	L2	203	BCR	C30-C25-C26	-2.24	119.44	122.59
14	M2	1201	CLA	O2D-CGD-O1D	-2.24	119.37	123.82
16	A6	1643	BCR	C33-C5-C4	-2.24	109.32	113.56
16	B1	847	BCR	C30-C25-C26	-2.24	119.44	122.59
14	B6	826	CLA	CMB-C2B-C1B	-2.24	125.02	128.46
16	J5	103	BCR	C12-C13-C14	-2.24	115.50	118.94
16	L3	206	BCR	C24-C25-C26	-2.24	116.20	121.54
14	A6	1608	CLA	CBC-CAC-C3C	-2.24	106.18	112.42
14	B4	824	CLA	CHD-C4C-C3C	-2.24	121.58	124.88
14	B3	1814	CLA	CHD-C4C-C3C	-2.24	121.58	124.88
14	B6	820	CLA	O2A-CGA-O1A	-2.24	118.12	123.58
14	L5	202	CLA	O2D-CGD-O1D	-2.24	119.38	123.82
14	B5	1804	CLA	O2A-CGA-O1A	-2.24	118.12	123.58
16	J4	103	BCR	C38-C26-C27	-2.24	109.33	113.56
14	B2	840	CLA	C4C-C3C-C2C	-2.24	103.58	106.90
14	B1	801	CLA	O2D-CGD-O1D	-2.24	119.38	123.82
16	I2	101	BCR	C1-C6-C5	-2.24	119.45	122.59
14	A3	824	CLA	O2A-CGA-O1A	-2.24	118.12	123.58
14	A5	801	CLA	C1C-C2C-C3C	-2.24	104.54	106.93
15	B4	844	PQN	C17-C16-C15	-2.23	107.09	113.17
14	A6	1632	CLA	CHD-C4C-C3C	-2.23	121.58	124.88
14	A6	1614	CLA	CHD-C4C-C3C	-2.23	121.58	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1636	CLA	O1D-CGD-CBD	-2.23	120.44	124.58
14	B1	817	CLA	O2A-CGA-O1A	-2.23	118.13	123.58
16	A4	849	BCR	C33-C5-C4	-2.23	109.34	113.56
14	A4	808	CLA	O2A-CGA-O1A	-2.23	118.13	123.58
14	B1	823	CLA	CHD-C4C-C3C	-2.23	121.59	124.88
14	B6	820	CLA	CHD-C4C-C3C	-2.23	121.59	124.88
14	B3	1826	CLA	O1D-CGD-CBD	-2.23	120.44	124.58
14	A5	828	CLA	O2A-CGA-O1A	-2.23	118.14	123.58
14	A6	1622	CLA	O1D-CGD-CBD	-2.23	120.44	124.58
14	A1	813	CLA	O1D-CGD-CBD	-2.23	120.44	124.58
14	B6	816	CLA	O2A-CGA-O1A	-2.23	118.14	123.58
14	B4	812	CLA	CHD-C4C-C3C	-2.23	121.59	124.88
14	A3	830	CLA	O2A-CGA-O1A	-2.23	118.14	123.58
14	A5	802	CLA	OBD-CAD-CBD	-2.23	122.64	125.91
14	F2	202	CLA	CHD-C4C-C3C	-2.23	121.59	124.88
14	B4	830	CLA	CHD-C4C-C3C	-2.23	121.59	124.88
14	A5	816	CLA	CBC-CAC-C3C	-2.23	106.22	112.42
14	A6	1640	CLA	C4C-C3C-C2C	-2.23	103.60	106.90
14	B5	1822	CLA	O2A-CGA-O1A	-2.23	118.15	123.58
14	A6	1651	CLA	OBD-CAD-CBD	-2.23	122.64	125.91
14	A2	1632	CLA	O1D-CGD-CBD	-2.23	120.45	124.58
14	A4	835	CLA	O1D-CGD-CBD	-2.23	120.45	124.58
14	K3	1401	CLA	CHD-C4C-C3C	-2.23	121.60	124.88
14	A5	838	CLA	CHD-C4C-C3C	-2.23	121.60	124.88
14	B5	1824	CLA	CHD-C4C-C3C	-2.23	121.60	124.88
16	A1	846	BCR	C1-C6-C5	-2.23	119.46	122.59
16	J1	103	BCR	C1-C6-C5	-2.23	119.46	122.59
16	B4	848	BCR	C19-C18-C17	-2.22	115.53	118.94
14	B3	1836	CLA	CHD-C4C-C3C	-2.22	121.60	124.88
14	A4	811	CLA	O2D-CGD-O1D	-2.22	119.41	123.82
16	M1	1202	BCR	C33-C5-C4	-2.22	109.36	113.56
14	M1	1201	CLA	O1D-CGD-CBD	-2.22	120.46	124.58
16	M3	1602	BCR	C33-C5-C4	-2.22	109.36	113.56
16	A1	847	BCR	C33-C5-C4	-2.22	109.36	113.56
15	B5	1844	PQN	C17-C16-C15	-2.22	107.12	113.17
14	M6	1201	CLA	O2D-CGD-O1D	-2.22	119.41	123.82
16	J5	103	BCR	C1-C6-C5	-2.22	119.47	122.59
14	B6	824	CLA	CHD-C4C-C3C	-2.22	121.60	124.88
14	B4	822	CLA	CHD-C4C-C3C	-2.22	121.60	124.88
16	F4	203	BCR	C33-C5-C4	-2.22	109.36	113.56
16	B1	846	BCR	C19-C18-C17	-2.22	115.53	118.94
14	A3	833	CLA	CBC-CAC-C3C	-2.22	106.24	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	809	CLA	O2A-CGA-O1A	-2.22	118.16	123.58
14	A4	831	CLA	C1C-C2C-C3C	-2.22	104.55	106.93
14	B5	1812	CLA	CHD-C4C-C3C	-2.22	121.60	124.88
14	A6	1632	CLA	C1C-C2C-C3C	-2.22	104.55	106.93
14	B1	819	CLA	O2A-CGA-O1A	-2.22	118.16	123.58
14	A1	831	CLA	CBC-CAC-C3C	-2.22	106.24	112.42
14	A4	811	CLA	O2A-CGA-O1A	-2.22	118.17	123.58
14	B1	801	CLA	CHD-C4C-C3C	-2.22	121.61	124.88
16	M5	101	BCR	C33-C5-C4	-2.22	109.37	113.56
14	A4	837	CLA	CHD-C4C-C3C	-2.22	121.61	124.88
16	A5	845	BCR	C38-C26-C27	-2.22	109.37	113.56
14	B3	1829	CLA	C1C-C2C-C3C	-2.22	104.56	106.93
16	L1	209	BCR	C33-C5-C4	-2.22	109.37	113.56
16	A3	847	BCR	C33-C5-C4	-2.22	109.37	113.56
14	A6	1630	CLA	O1D-CGD-CBD	-2.22	120.47	124.58
14	A4	807	CLA	O2A-CGA-O1A	-2.22	118.17	123.58
14	B4	815	CLA	O2A-CGA-O1A	-2.22	118.17	123.58
14	A4	827	CLA	O2A-CGA-O1A	-2.22	118.17	123.58
16	L6	201	BCR	C33-C5-C4	-2.22	109.37	113.56
14	A1	814	CLA	O1D-CGD-CBD	-2.22	120.47	124.58
16	M2	1202	BCR	C7-C6-C5	-2.22	116.26	121.54
16	I1	103	BCR	C38-C26-C27	-2.21	109.38	113.56
14	B2	812	CLA	CHD-C4C-C3C	-2.21	121.61	124.88
14	A1	838	CLA	O2A-CGA-O1A	-2.21	118.18	123.58
14	A2	1640	CLA	CHD-C4C-C3C	-2.21	121.62	124.88
16	I1	102	BCR	C1-C6-C5	-2.21	119.48	122.59
14	M1	1201	CLA	O2D-CGD-O1D	-2.21	119.43	123.82
14	A4	813	CLA	CHD-C4C-C3C	-2.21	121.62	124.88
14	B6	802	CLA	OBD-CAD-CBD	-2.21	122.66	125.91
14	A2	1634	CLA	C1C-C2C-C3C	-2.21	104.56	106.93
16	J3	103	BCR	C1-C6-C5	-2.21	119.48	122.59
14	B6	810	CLA	O2A-CGA-O1A	-2.21	118.19	123.58
14	M6	1201	CLA	CBC-CAC-C3C	-2.21	106.27	112.42
14	B3	1826	CLA	CHD-C4C-C3C	-2.21	121.62	124.88
14	A2	1633	CLA	CHD-C4C-C3C	-2.21	121.62	124.88
16	A1	842	BCR	C38-C26-C27	-2.21	109.38	113.56
14	J6	1101	CLA	CHD-C4C-C3C	-2.21	121.62	124.88
14	A4	830	CLA	CHD-C4C-C3C	-2.21	121.62	124.88
14	A6	1631	CLA	O2A-CGA-O1A	-2.21	118.19	123.58
16	B1	843	BCR	C33-C5-C4	-2.21	109.39	113.56
16	A2	1647	BCR	C33-C5-C4	-2.21	109.39	113.56
16	L1	203	BCR	C30-C25-C26	-2.21	119.49	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B5	1847	BCR	C30-C25-C26	-2.21	119.49	122.59
14	A5	820	CLA	O2A-CGA-O1A	-2.21	118.19	123.58
16	A5	846	BCR	C30-C25-C26	-2.21	119.49	122.59
14	A6	1615	CLA	CHD-C4C-C3C	-2.21	121.62	124.88
14	B1	809	CLA	O1D-CGD-CBD	-2.21	120.49	124.58
14	L3	203	CLA	C12-C11-C10	-2.21	102.76	113.23
14	L1	205	CLA	O2A-CGA-O1A	-2.21	118.20	123.58
14	B2	812	CLA	O2A-CGA-O1A	-2.20	118.20	123.58
14	B6	828	CLA	CHD-C4C-C3C	-2.20	121.63	124.88
14	J4	101	CLA	CHD-C4C-C3C	-2.20	121.63	124.88
14	B3	1805	CLA	C12-C11-C10	-2.20	102.78	113.23
14	B1	802	CLA	CBC-CAC-C3C	-2.20	106.29	112.42
14	B4	819	CLA	CHD-C4C-C3C	-2.20	121.63	124.88
16	J1	104	BCR	C19-C18-C17	-2.20	115.56	118.94
14	B5	1829	CLA	O2A-CGA-O1A	-2.20	118.21	123.58
14	B3	1831	CLA	C1C-C2C-C3C	-2.20	104.57	106.93
14	A6	1631	CLA	CHD-C4C-C3C	-2.20	121.63	124.88
14	A3	802	CLA	CHD-C4C-C3C	-2.20	121.63	124.88
14	A2	1603	CLA	OBD-CAD-CBD	-2.20	122.68	125.91
14	A3	843	CLA	C1C-C2C-C3C	-2.20	104.57	106.93
14	B4	806	CLA	O1D-CGD-CBD	-2.20	120.50	124.58
14	B4	840	CLA	CHD-C4C-C3C	-2.20	121.63	124.88
14	A6	1612	CLA	CHD-C4C-C3C	-2.20	121.63	124.88
14	B1	805	CLA	OBD-CAD-CBD	-2.20	122.68	125.91
14	A2	1608	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
14	L4	201	CLA	O2D-CGD-O1D	-2.20	119.46	123.82
16	A2	1652	BCR	C33-C5-C4	-2.20	109.41	113.56
14	B2	839	CLA	C4C-C3C-C2C	-2.20	103.64	106.90
14	A2	1605	CLA	CHD-C4C-C3C	-2.20	121.64	124.88
14	B6	813	CLA	CHD-C4C-C3C	-2.20	121.64	124.88
14	B5	1818	CLA	O2A-CGA-O1A	-2.20	118.22	123.58
14	B3	1839	CLA	O2A-CGA-O1A	-2.20	118.22	123.58
14	A2	1603	CLA	CBC-CAC-C3C	-2.20	106.30	112.42
14	A3	820	CLA	O2A-CGA-O1A	-2.20	118.22	123.58
14	A6	1624	CLA	CHD-C4C-C3C	-2.20	121.64	124.88
14	B5	1803	CLA	CHD-C4C-C3C	-2.20	121.64	124.88
14	F2	204	CLA	CHD-C4C-C3C	-2.20	121.64	124.88
14	A3	841	CLA	O2A-CGA-O1A	-2.20	118.22	123.58
16	A2	1648	BCR	C30-C25-C26	-2.20	119.50	122.59
16	A5	849	BCR	C1-C6-C5	-2.20	119.50	122.59
14	J2	101	CLA	CHD-C4C-C3C	-2.20	121.64	124.88
14	B5	1833	CLA	O2A-CGA-O1A	-2.20	118.22	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A1	801	CLA	C1C-C2C-C3C	-2.20	104.58	106.93
16	M4	101	BCR	C7-C6-C5	-2.20	116.31	121.54
14	M6	1201	CLA	O1D-CGD-CBD	-2.20	120.51	124.58
16	I5	102	BCR	C30-C25-C26	-2.20	119.51	122.59
14	L5	205	CLA	O2A-CGA-O1A	-2.20	118.22	123.58
14	B3	1822	CLA	CHD-C4C-C3C	-2.19	121.64	124.88
14	A2	1610	CLA	CBC-CAC-C3C	-2.19	106.31	112.42
16	J3	104	BCR	C19-C18-C17	-2.19	115.57	118.94
14	L3	203	CLA	O2A-CGA-O1A	-2.19	118.23	123.58
14	A2	1616	CLA	CHD-C4C-C3C	-2.19	121.64	124.88
14	B5	1829	CLA	C1C-C2C-C3C	-2.19	104.58	106.93
14	A5	841	CLA	C4C-C3C-C2C	-2.19	103.65	106.90
16	B4	847	BCR	C30-C25-C26	-2.19	119.51	122.59
16	B2	846	BCR	C19-C18-C17	-2.19	115.58	118.94
14	A3	840	CLA	O2A-CGA-O1A	-2.19	118.23	123.58
14	B4	815	CLA	C4C-C3C-C2C	-2.19	103.65	106.90
14	L4	204	CLA	O2A-CGA-O1A	-2.19	118.23	123.58
14	B3	1812	CLA	O2A-CGA-O1A	-2.19	118.23	123.58
14	B5	1826	CLA	O1D-CGD-CBD	-2.19	120.52	124.58
16	A3	850	BCR	C1-C6-C5	-2.19	119.51	122.59
14	J1	101	CLA	CHD-C4C-C3C	-2.19	121.65	124.88
14	B4	829	CLA	O2A-CGA-O1A	-2.19	118.24	123.58
16	B1	845	BCR	C30-C25-C26	-2.19	119.51	122.59
16	L6	204	BCR	C30-C25-C26	-2.19	119.51	122.59
14	B5	1803	CLA	C12-C11-C10	-2.19	102.84	113.23
16	A6	1643	BCR	C38-C26-C27	-2.19	109.43	113.56
14	A1	807	CLA	CBC-CAC-C3C	-2.19	106.33	112.42
14	A6	1612	CLA	O2D-CGD-O1D	-2.19	119.48	123.82
14	A4	812	CLA	CHD-C4C-C3C	-2.19	121.65	124.88
16	A4	846	BCR	C38-C26-C27	-2.19	109.43	113.56
14	B4	828	CLA	C4C-C3C-C2C	-2.19	103.66	106.90
14	L6	202	CLA	C1C-C2C-C3C	-2.19	104.59	106.93
14	A3	801	CLA	C1C-C2C-C3C	-2.19	104.59	106.93
14	J6	1103	CLA	CHD-C4C-C3C	-2.19	121.66	124.88
14	B2	837	CLA	CHD-C4C-C3C	-2.19	121.66	124.88
14	B1	801	CLA	CBC-CAC-C3C	-2.19	106.34	112.42
14	A6	1604	CLA	O2A-CGA-O1A	-2.18	118.25	123.58
15	B6	842	PQN	C17-C16-C15	-2.18	107.23	113.17
14	A1	835	CLA	CHD-C4C-C3C	-2.18	121.66	124.88
14	B3	1842	CLA	C4C-C3C-C2C	-2.18	103.66	106.90
16	B2	844	BCR	C30-C25-C26	-2.18	119.52	122.59
14	A3	838	CLA	CHD-C4C-C3C	-2.18	121.66	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	836	CLA	O2D-CGD-O1D	-2.18	119.49	123.82
16	L5	201	BCR	C33-C5-C4	-2.18	109.44	113.56
14	B3	1839	CLA	O1D-CGD-CBD	-2.18	120.54	124.58
14	A3	833	CLA	CHD-C4C-C3C	-2.18	121.66	124.88
16	L6	201	BCR	C1-C6-C5	-2.18	119.53	122.59
14	B2	825	CLA	O1D-CGD-CBD	-2.18	120.54	124.58
14	A4	840	CLA	O2A-CGA-O1A	-2.18	118.26	123.58
14	M2	1201	CLA	O2A-CGA-O1A	-2.18	118.26	123.58
14	A5	802	CLA	CBC-CAC-C3C	-2.18	106.36	112.42
16	J1	104	BCR	C12-C13-C14	-2.18	115.60	118.94
14	A4	829	CLA	O1D-CGD-CBD	-2.18	120.54	124.58
16	A1	844	BCR	C38-C26-C27	-2.18	109.45	113.56
14	B2	828	CLA	O2A-CGA-O1A	-2.18	118.27	123.58
14	B1	802	CLA	CHD-C4C-C3C	-2.18	121.67	124.88
14	B4	842	CLA	C12-C11-C10	-2.18	102.90	113.23
14	B5	1807	CLA	OBD-CAD-CBD	-2.18	122.72	125.91
14	A1	829	CLA	O2A-CGA-O1A	-2.18	118.27	123.58
16	A1	847	BCR	C34-C9-C10	-2.18	119.88	122.92
14	A5	818	CLA	O2A-CGA-O1A	-2.18	118.27	123.58
16	L2	201	BCR	C33-C5-C4	-2.18	109.45	113.56
16	J6	1104	BCR	C1-C6-C5	-2.18	119.53	122.59
14	B3	1802	CLA	CHD-C4C-C3C	-2.17	121.67	124.88
14	B3	1824	CLA	CHD-C4C-C3C	-2.17	121.67	124.88
14	B1	829	CLA	C4-C3-C5	-2.17	111.54	115.29
14	A4	823	CLA	CHD-C4C-C3C	-2.17	121.67	124.88
14	B1	830	CLA	CHD-C4C-C3C	-2.17	121.67	124.88
16	I1	103	BCR	C19-C18-C17	-2.17	115.61	118.94
14	B5	1834	CLA	O1D-CGD-CBD	-2.17	120.55	124.58
14	A4	805	CLA	CMB-C2B-C1B	-2.17	125.12	128.46
14	B4	831	CLA	CHD-C4C-C3C	-2.17	121.68	124.88
14	B4	801	CLA	CBC-CAC-C3C	-2.17	106.38	112.42
14	B4	841	CLA	O2D-CGD-O1D	-2.17	119.51	123.82
14	B6	822	CLA	CHD-C4C-C3C	-2.17	121.68	124.88
14	A6	1651	CLA	CBC-CAC-C3C	-2.17	106.38	112.42
16	B3	1848	BCR	C19-C18-C17	-2.17	115.61	118.94
14	B4	831	CLA	C1C-C2C-C3C	-2.17	104.61	106.93
14	L1	201	CLA	C1C-C2C-C3C	-2.17	104.61	106.93
16	L2	208	BCR	C19-C18-C17	-2.17	115.61	118.94
14	A4	824	CLA	O1D-CGD-CBD	-2.17	120.56	124.58
14	A4	820	CLA	CHD-C4C-C3C	-2.17	121.68	124.88
14	B1	822	CLA	OBD-CAD-CBD	-2.17	122.72	125.91
14	K1	1401	CLA	O2D-CGD-O1D	-2.17	119.52	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1605	CLA	CHD-C4C-C3C	-2.17	121.68	124.88
16	B6	850	BCR	C30-C25-C26	-2.17	119.54	122.59
14	B3	1828	CLA	C4C-C3C-C2C	-2.17	103.69	106.90
14	B5	1811	CLA	C1C-C2C-C3C	-2.17	104.61	106.93
14	B6	825	CLA	CHD-C4C-C3C	-2.17	121.68	124.88
14	B3	1808	CLA	CHD-C4C-C3C	-2.17	121.68	124.88
14	B1	814	CLA	O2A-CGA-O1A	-2.17	118.29	123.58
14	A3	804	CLA	C12-C11-C10	-2.17	106.01	113.59
14	A5	802	CLA	CHD-C4C-C3C	-2.17	121.68	124.88
14	B3	1828	CLA	O1D-CGD-CBD	-2.17	120.56	124.58
16	A6	1645	BCR	C38-C26-C27	-2.17	109.47	113.56
16	B5	1845	BCR	C33-C5-C4	-2.17	109.47	113.56
14	A5	812	CLA	O2A-CGA-O1A	-2.17	118.30	123.58
14	B4	831	CLA	O2A-CGA-O1A	-2.17	118.30	123.58
14	A3	832	CLA	C1C-C2C-C3C	-2.17	104.61	106.93
14	A3	842	CLA	C4C-C3C-C2C	-2.16	103.69	106.90
14	B6	840	CLA	C4C-C3C-C2C	-2.16	103.69	106.90
14	B6	817	CLA	CHD-C4C-C3C	-2.16	121.69	124.88
14	A4	811	CLA	CHD-C4C-C3C	-2.16	121.69	124.88
14	A5	831	CLA	CHD-C4C-C3C	-2.16	121.69	124.88
16	L2	208	BCR	C38-C26-C27	-2.16	109.47	113.56
14	B4	820	CLA	O2A-CGA-O1A	-2.16	118.30	123.58
14	B3	1822	CLA	O2A-CGA-O1A	-2.16	118.30	123.58
14	B1	854	CLA	O2A-CGA-O1A	-2.16	118.30	123.58
14	A1	812	CLA	O2A-CGA-O1A	-2.16	118.30	123.58
16	L4	208	BCR	C1-C6-C5	-2.16	119.55	122.59
14	A6	1637	CLA	CHD-C4C-C3C	-2.16	121.69	124.88
14	A4	830	CLA	O2A-CGA-O1A	-2.16	118.31	123.58
14	A5	821	CLA	C12-C11-C10	-2.16	102.97	113.23
16	B6	846	BCR	C19-C18-C17	-2.16	115.62	118.94
14	B1	840	CLA	O2A-CGA-O1A	-2.16	118.31	123.58
14	B3	1830	CLA	CHD-C4C-C3C	-2.16	121.69	124.88
14	J1	102	CLA	CHD-C4C-C3C	-2.16	121.69	124.88
14	B4	842	CLA	C4C-C3C-C2C	-2.16	103.70	106.90
14	A6	1602	CLA	C1C-C2C-C3C	-2.16	104.62	106.93
14	A5	814	CLA	CHD-C4C-C3C	-2.16	121.69	124.88
14	B5	1802	CLA	CHD-C4C-C3C	-2.16	121.69	124.88
14	B1	818	CLA	O2A-CGA-O1A	-2.16	118.31	123.58
14	L6	208	CLA	O1D-CGD-CBD	-2.16	120.58	124.58
14	B2	836	CLA	O2A-CGA-O1A	-2.16	118.31	123.58
14	B6	834	CLA	O2D-CGD-O1D	-2.16	119.54	123.82
14	A6	1632	CLA	CBC-CAC-C3C	-2.16	106.41	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A2	1602	CLA	C1C-C2C-C3C	-2.16	104.62	106.93
14	A4	807	CLA	CBC-CAC-C3C	-2.16	106.42	112.42
14	B5	1809	CLA	O2D-CGD-O1D	-2.16	119.54	123.82
14	L6	206	CLA	O2A-CGA-O1A	-2.16	118.32	123.58
14	A2	1607	CLA	CAA-C2A-C3A	-2.16	106.90	112.81
14	A6	1640	CLA	C12-C11-C10	-2.16	103.00	113.23
14	B4	812	CLA	O2A-CGA-O1A	-2.16	118.32	123.58
14	B3	1831	CLA	CHD-C4C-C3C	-2.16	121.70	124.88
14	B4	828	CLA	O1D-CGD-CBD	-2.16	120.58	124.58
16	L2	201	BCR	C1-C6-C5	-2.16	119.56	122.59
16	I1	103	BCR	C30-C25-C26	-2.15	119.56	122.59
14	B3	1804	CLA	O1D-CGD-CBD	-2.15	120.59	124.58
14	A4	836	CLA	CHD-C4C-C3C	-2.15	121.70	124.88
14	B4	806	CLA	O2D-CGD-O1D	-2.15	119.55	123.82
14	A3	805	CLA	CAA-C2A-C3A	-2.15	106.91	112.81
16	L2	203	BCR	C12-C13-C14	-2.15	115.64	118.94
14	B1	821	CLA	O2D-CGD-O1D	-2.15	119.55	123.82
14	A2	1630	CLA	C1C-C2C-C3C	-2.15	104.63	106.93
16	L4	208	BCR	C33-C5-C4	-2.15	109.50	113.56
14	L3	202	CLA	O2D-CGD-O1D	-2.15	119.55	123.82
14	B6	831	CLA	O2D-CGD-O1D	-2.15	119.55	123.82
14	B2	802	CLA	CBC-CAC-C3C	-2.15	106.43	112.42
16	L3	206	BCR	C19-C18-C17	-2.15	115.64	118.94
16	A5	847	BCR	C38-C26-C27	-2.15	109.50	113.56
16	A6	1652	BCR	C1-C6-C5	-2.15	119.57	122.59
16	L4	206	BCR	C30-C25-C26	-2.15	119.57	122.59
16	F4	204	BCR	C30-C25-C26	-2.15	119.57	122.59
14	B2	825	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
14	A3	814	CLA	O1D-CGD-CBD	-2.15	120.59	124.58
16	L5	207	BCR	C38-C26-C27	-2.15	109.50	113.56
14	A3	805	CLA	O1D-CGD-CBD	-2.15	120.59	124.58
14	B5	1808	CLA	CHD-C4C-C3C	-2.15	121.71	124.88
14	B1	841	CLA	C4C-C3C-C2C	-2.15	103.72	106.90
14	J6	1101	CLA	O1D-CGD-CBD	-2.15	120.60	124.58
14	A5	803	CLA	CHD-C4C-C3C	-2.15	121.71	124.88
14	A2	1641	CLA	O2A-CGA-O1A	-2.15	118.34	123.58
16	A3	849	BCR	C38-C26-C27	-2.15	109.50	113.56
14	A4	832	CLA	CBC-CAC-C3C	-2.15	106.44	112.42
16	J3	104	BCR	C30-C25-C26	-2.15	119.57	122.59
14	B2	833	CLA	CHD-C4C-C3C	-2.15	121.71	124.88
14	A3	819	CLA	CHD-C4C-C3C	-2.15	121.71	124.88
16	A2	1649	BCR	C38-C26-C27	-2.15	109.51	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I4	102	BCR	C12-C13-C14	-2.15	115.65	118.94
14	M6	1201	CLA	O2A-CGA-O1A	-2.14	118.35	123.58
16	B3	1848	BCR	C38-C26-C27	-2.14	109.51	113.56
14	B1	826	CLA	CHD-C4C-C3C	-2.14	121.72	124.88
16	A4	847	BCR	C1-C6-C5	-2.14	119.58	122.59
14	B6	838	CLA	O2A-CGA-O1A	-2.14	118.35	123.58
16	I3	102	BCR	C12-C13-C14	-2.14	115.65	118.94
14	B5	1805	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
14	A2	1633	CLA	O2A-CGA-O1A	-2.14	118.35	123.58
14	K5	101	CLA	CHD-C4C-C3C	-2.14	121.72	124.88
16	J4	104	BCR	C19-C18-C17	-2.14	115.65	118.94
14	L5	203	CLA	O2A-CGA-O1A	-2.14	118.35	123.58
16	J2	103	BCR	C24-C25-C26	-2.14	116.43	121.54
14	B1	833	CLA	O2D-CGD-O1D	-2.14	119.57	123.82
14	A2	1614	CLA	O2A-CGA-O1A	-2.14	118.36	123.58
16	J2	103	BCR	C19-C18-C17	-2.14	115.66	118.94
14	B1	827	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
16	A6	1646	BCR	C1-C6-C5	-2.14	119.58	122.59
16	B1	847	BCR	C19-C18-C17	-2.14	115.66	118.94
14	B2	833	CLA	O2D-CGD-O1D	-2.14	119.58	123.82
14	B2	808	CLA	C1C-C2C-C3C	-2.14	104.64	106.93
16	A5	850	BCR	C34-C9-C10	-2.14	119.93	122.92
14	A3	812	CLA	CHD-C4C-C3C	-2.14	121.73	124.88
14	B2	805	CLA	CHD-C4C-C3C	-2.14	121.73	124.88
14	A2	1615	CLA	CHD-C4C-C3C	-2.14	121.73	124.88
14	B4	840	CLA	O1D-CGD-CBD	-2.14	120.62	124.58
14	B1	839	CLA	O1D-CGD-CBD	-2.14	120.62	124.58
16	I4	102	BCR	C30-C25-C26	-2.14	119.59	122.59
14	L5	206	CLA	O2D-CGD-O1D	-2.14	119.58	123.82
14	B2	825	CLA	C4C-C3C-C2C	-2.14	103.73	106.90
14	A2	1645	CLA	CHD-C4C-C3C	-2.14	121.73	124.88
14	A1	821	CLA	O2A-CGA-O1A	-2.14	118.37	123.58
16	B3	1851	BCR	C30-C25-C26	-2.13	119.59	122.59
16	A4	848	BCR	C1-C6-C5	-2.13	119.59	122.59
16	A4	844	BCR	C33-C5-C4	-2.13	109.53	113.56
14	B4	805	CLA	C12-C11-C10	-2.13	103.10	113.23
14	A6	1633	CLA	O2D-CGD-O1D	-2.13	119.58	123.82
16	L4	206	BCR	C19-C18-C17	-2.13	115.67	118.94
14	J2	101	CLA	O2D-CGD-O1D	-2.13	119.59	123.82
14	A5	833	CLA	CBC-CAC-C3C	-2.13	106.48	112.42
16	L6	209	BCR	C38-C26-C27	-2.13	109.53	113.56
16	L4	206	BCR	C38-C26-C27	-2.13	109.53	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1828	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
14	B4	805	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
14	A3	828	CLA	O2A-CGA-O1A	-2.13	118.38	123.58
16	B2	850	BCR	C30-C25-C26	-2.13	119.59	122.59
14	A6	1620	CLA	O2A-CGA-O1A	-2.13	118.38	123.58
14	B2	828	CLA	CHD-C4C-C3C	-2.13	121.74	124.88
14	B3	1834	CLA	O2D-CGD-O1D	-2.13	119.59	123.82
14	B3	1827	CLA	CHD-C4C-C3C	-2.13	121.74	124.88
14	B3	1820	CLA	CHD-C4C-C3C	-2.13	121.74	124.88
14	J5	102	CLA	CHD-C4C-C3C	-2.13	121.74	124.88
16	A6	1644	BCR	C30-C25-C26	-2.13	119.60	122.59
16	J1	104	BCR	C24-C25-C26	-2.13	116.46	121.54
16	L3	206	BCR	C30-C25-C26	-2.13	119.60	122.59
14	A2	1625	CLA	O2D-CGD-O1D	-2.13	119.59	123.82
16	I5	102	BCR	C38-C26-C27	-2.13	109.54	113.56
14	B5	1836	CLA	CHD-C4C-C3C	-2.13	121.74	124.88
16	B5	1849	BCR	C30-C25-C26	-2.13	119.60	122.59
14	B4	804	CLA	O2A-CGA-O1A	-2.13	118.39	123.58
14	A1	804	CLA	CAA-C2A-C3A	-2.13	106.97	112.81
14	A4	802	CLA	CHD-C4C-C3C	-2.13	121.74	124.88
16	B5	1849	BCR	C19-C18-C17	-2.13	115.67	118.94
14	B5	1805	CLA	C12-C11-C10	-2.13	103.13	113.23
14	B1	828	CLA	O1D-CGD-CBD	-2.13	120.63	124.58
16	F5	1302	BCR	C30-C25-C26	-2.13	119.60	122.59
14	J4	102	CLA	CHD-C4C-C3C	-2.13	121.74	124.88
14	A5	812	CLA	CHD-C4C-C3C	-2.13	121.74	124.88
14	B2	821	CLA	CHD-C4C-C3C	-2.13	121.74	124.88
14	B2	831	CLA	C12-C11-C10	-2.13	103.14	113.23
14	A3	834	CLA	O2A-CGA-O1A	-2.13	118.39	123.58
14	B1	808	CLA	CHD-C4C-C3C	-2.13	121.75	124.88
16	I3	101	BCR	C1-C6-C5	-2.12	119.61	122.59
14	A1	803	CLA	C12-C11-C10	-2.12	106.16	113.59
16	A5	850	BCR	C12-C13-C14	-2.12	115.68	118.94
14	B5	1801	CLA	O2A-CGA-O1A	-2.12	118.40	123.58
14	B3	1803	CLA	CBC-CAC-C3C	-2.12	106.51	112.42
14	A6	1638	CLA	O1D-CGD-CBD	-2.12	120.64	124.58
14	B4	822	CLA	O2A-CGA-O1A	-2.12	118.40	123.58
14	A3	822	CLA	O2A-CGA-O1A	-2.12	118.40	123.58
14	A2	1614	CLA	CHD-C4C-C3C	-2.12	121.75	124.88
14	A3	833	CLA	C1C-C2C-C3C	-2.12	104.66	106.93
14	A3	804	CLA	O2A-CGA-O1A	-2.12	118.40	123.58
14	A6	1619	CLA	CHD-C4C-C3C	-2.12	121.75	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1815	CLA	CHD-C4C-C3C	-2.12	121.75	124.88
14	A1	803	CLA	O2D-CGD-O1D	-2.12	119.61	123.82
14	A3	803	CLA	O1D-CGD-CBD	-2.12	120.64	124.58
14	B1	840	CLA	O2D-CGD-O1D	-2.12	119.61	123.82
14	B2	815	CLA	O1D-CGD-CBD	-2.12	120.65	124.58
14	A3	812	CLA	O2A-CGA-O1A	-2.12	118.41	123.58
14	A1	808	CLA	O2A-CGA-O1A	-2.12	118.41	123.58
14	A2	1603	CLA	CHD-C4C-C3C	-2.12	121.75	124.88
14	A3	816	CLA	O2A-CGA-O1A	-2.12	118.41	123.58
14	B3	1836	CLA	O2D-CGD-O1D	-2.12	119.61	123.82
14	J6	1102	CLA	CHD-C4C-C3C	-2.12	121.75	124.88
14	B4	814	CLA	CHD-C4C-C3C	-2.12	121.75	124.88
14	B6	829	CLA	O2A-CGA-O1A	-2.12	118.41	123.58
14	B3	1829	CLA	O1D-CGD-CBD	-2.12	120.65	124.58
14	B1	819	CLA	CHD-C4C-C3C	-2.12	121.75	124.88
16	F4	203	BCR	C30-C25-C26	-2.12	119.61	122.59
14	A2	1644	CLA	C1C-C2C-C3C	-2.12	104.66	106.93
14	B1	833	CLA	C12-C11-C10	-2.12	103.19	113.23
14	A6	1622	CLA	O2A-CGA-O1A	-2.12	118.42	123.58
16	A6	1648	BCR	C1-C6-C5	-2.12	119.62	122.59
14	A1	811	CLA	O2A-CGA-O1A	-2.12	118.42	123.58
14	B4	808	CLA	CHD-C4C-C3C	-2.12	121.76	124.88
14	B4	834	CLA	C12-C11-C10	-2.12	103.19	113.23
16	A5	845	BCR	C33-C5-C4	-2.12	109.56	113.56
14	A5	835	CLA	O1D-CGD-CBD	-2.12	120.66	124.58
14	A1	840	CLA	CHD-C4C-C3C	-2.12	121.76	124.88
14	A1	802	CLA	CHD-C4C-C3C	-2.12	121.76	124.88
16	L6	204	BCR	C12-C13-C14	-2.11	115.70	118.94
16	L6	209	BCR	C19-C18-C17	-2.11	115.70	118.94
14	B3	1815	CLA	C4C-C3C-C2C	-2.11	103.77	106.90
16	A3	851	BCR	C1-C6-C5	-2.11	119.62	122.59
14	B6	832	CLA	O1D-CGD-CBD	-2.11	120.66	124.58
14	A3	805	CLA	CHD-C4C-C3C	-2.11	121.76	124.88
16	J5	104	BCR	C19-C18-C17	-2.11	115.70	118.94
14	B1	806	CLA	C12-C11-C10	-2.11	103.20	113.23
14	B6	806	CLA	O1D-CGD-CBD	-2.11	120.66	124.58
14	B6	827	CLA	O2A-CGA-O1A	-2.11	118.42	123.58
14	A6	1636	CLA	CHC-C1C-C2C	-2.11	120.87	126.75
14	A3	824	CLA	CHD-C4C-C3C	-2.11	121.76	124.88
14	A5	838	CLA	O2D-CGD-O1D	-2.11	119.63	123.82
14	A1	831	CLA	C1C-C2C-C3C	-2.11	104.67	106.93
14	B1	854	CLA	CHC-C1C-C2C	-2.11	120.87	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B6	847	BCR	C15-C16-C17	-2.11	118.95	123.46
14	L5	204	CLA	O2A-CGA-O1A	-2.11	118.43	123.58
16	B3	1849	BCR	C30-C25-C26	-2.11	119.62	122.59
14	A3	811	CLA	O2A-CGA-O1A	-2.11	118.43	123.58
14	B1	835	CLA	CHD-C4C-C3C	-2.11	121.77	124.88
16	A1	842	BCR	C33-C5-C4	-2.11	109.57	113.56
16	B6	845	BCR	C38-C26-C27	-2.11	109.57	113.56
16	A1	847	BCR	C1-C6-C5	-2.11	119.63	122.59
14	B4	803	CLA	CBC-CAC-C3C	-2.11	106.55	112.42
15	B2	841	PQN	C17-C16-C15	-2.11	107.43	113.17
14	A2	1605	CLA	O1D-CGD-CBD	-2.11	120.67	124.58
14	B3	1843	CLA	C4C-C3C-C2C	-2.11	103.78	106.90
14	B1	821	CLA	O2A-CGA-O1A	-2.11	118.44	123.58
14	A2	1604	CLA	CHD-C4C-C3C	-2.11	121.77	124.88
14	B5	1840	CLA	O1D-CGD-CBD	-2.11	120.67	124.58
14	B6	809	CLA	C7-C6-C5	-2.11	107.44	113.17
14	B6	841	CLA	C4C-C3C-C2C	-2.11	103.78	106.90
14	A4	803	CLA	C12-C11-C10	-2.11	106.22	113.59
14	B5	1819	CLA	O2A-CGA-O1A	-2.11	118.44	123.58
14	A6	1613	CLA	CHD-C4C-C3C	-2.11	121.77	124.88
14	A1	822	CLA	CHD-C4C-C3C	-2.11	121.77	124.88
16	A3	852	BCR	C1-C6-C5	-2.10	119.63	122.59
16	B1	844	BCR	C33-C5-C4	-2.10	109.58	113.56
14	A6	1640	CLA	O2A-CGA-O1A	-2.10	118.44	123.58
14	B5	1812	CLA	CHC-C1C-C2C	-2.10	120.89	126.75
14	A2	1607	CLA	O1D-CGD-CBD	-2.10	120.68	124.58
14	B2	824	CLA	CHD-C4C-C3C	-2.10	121.78	124.88
14	B4	818	CLA	O1D-CGD-CBD	-2.10	120.68	124.58
14	A5	824	CLA	CHD-C4C-C3C	-2.10	121.78	124.88
16	A6	1647	BCR	C1-C6-C5	-2.10	119.64	122.59
16	A2	1652	BCR	C12-C13-C14	-2.10	115.71	118.94
14	B1	827	CLA	C7-C6-C5	-2.10	107.45	113.17
14	B5	1843	CLA	C4C-C3C-C2C	-2.10	103.78	106.90
16	A4	849	BCR	C1-C6-C5	-2.10	119.64	122.59
16	B2	847	BCR	C1-C6-C5	-2.10	119.64	122.59
14	B1	827	CLA	O2A-CGA-O1A	-2.10	118.45	123.58
14	B4	806	CLA	CBC-CAC-C3C	-2.10	106.57	112.42
14	A6	1623	CLA	O1D-CGD-CBD	-2.10	120.69	124.58
14	L2	206	CLA	O2A-CGA-O1A	-2.10	118.45	123.58
14	B6	817	CLA	O2A-CGA-O1A	-2.10	118.45	123.58
14	A2	1626	CLA	CHD-C4C-C3C	-2.10	121.78	124.88
14	B6	829	CLA	CHD-C4C-C3C	-2.10	121.78	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A5	806	CLA	CHD-C4C-C3C	-2.10	121.78	124.88
14	B5	1814	CLA	CHD-C4C-C3C	-2.10	121.78	124.88
14	A4	837	CLA	O2D-CGD-O1D	-2.10	119.66	123.82
14	A2	1643	CLA	C12-C11-C10	-2.10	103.28	113.23
14	B4	812	CLA	CHC-C1C-C2C	-2.10	120.91	126.75
14	A5	838	CLA	O1D-CGD-CBD	-2.10	120.69	124.58
14	A3	833	CLA	CHC-C1C-C2C	-2.10	120.91	126.75
14	A4	831	CLA	O2A-CGA-O1A	-2.10	118.47	123.58
14	B6	805	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
14	A1	802	CLA	O1D-CGD-CBD	-2.10	120.69	124.58
14	A2	1607	CLA	CHD-C4C-C3C	-2.10	121.79	124.88
14	A1	823	CLA	CHD-C4C-C3C	-2.10	121.79	124.88
16	B6	847	BCR	C1-C6-C5	-2.10	119.65	122.59
16	B3	1847	BCR	C38-C26-C27	-2.10	109.60	113.56
14	A3	821	CLA	CHD-C4C-C3C	-2.10	121.79	124.88
14	B5	1827	CLA	CHD-C4C-C3C	-2.10	121.79	124.88
16	J6	1105	BCR	C12-C13-C14	-2.10	115.73	118.94
14	B6	804	CLA	CBC-CAC-C3C	-2.10	106.59	112.42
14	A5	802	CLA	O2D-CGD-O1D	-2.09	119.66	123.82
16	J6	1105	BCR	C19-C18-C17	-2.09	115.73	118.94
16	L5	207	BCR	C19-C18-C17	-2.09	115.73	118.94
14	A5	841	CLA	C12-C11-C10	-2.09	103.29	113.23
14	L5	203	CLA	O2D-CGD-O1D	-2.09	119.67	123.82
14	A3	837	CLA	CHC-C1C-C2C	-2.09	120.92	126.75
14	B1	827	CLA	O1D-CGD-CBD	-2.09	120.70	124.58
14	B1	813	CLA	CHD-C4C-C3C	-2.09	121.79	124.88
14	A5	832	CLA	C1C-C2C-C3C	-2.09	104.69	106.93
14	B5	1828	CLA	O1D-CGD-CBD	-2.09	120.70	124.58
14	X2	1701	CLA	O1D-CGD-CBD	-2.09	120.70	124.58
14	A5	808	CLA	CBC-CAC-C3C	-2.09	106.60	112.42
14	A3	813	CLA	CHD-C4C-C3C	-2.09	121.79	124.88
14	B2	803	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
14	B4	801	CLA	CHD-C4C-C3C	-2.09	121.79	124.88
14	B4	833	CLA	O2D-CGD-O1D	-2.09	119.67	123.82
14	A5	802	CLA	C6-C5-C3	-2.09	107.75	112.82
14	B6	810	CLA	CHC-C1C-C2C	-2.09	120.93	126.75
14	B3	1812	CLA	CHC-C1C-C2C	-2.09	120.93	126.75
16	J5	104	BCR	C12-C13-C14	-2.09	115.73	118.94
14	A4	803	CLA	O2A-CGA-O1A	-2.09	118.48	123.58
14	B2	819	CLA	O2A-CGA-O1A	-2.09	118.48	123.58
14	A6	1632	CLA	CHC-C1C-C2C	-2.09	120.93	126.75
16	A3	856	BCR	C12-C13-C14	-2.09	115.74	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1828	CLA	O2A-CGA-O1A	-2.09	118.48	123.58
14	B4	841	CLA	C1C-C2C-C3C	-2.09	104.69	106.93
14	B3	1841	CLA	C1C-C2C-C3C	-2.09	104.69	106.93
14	A2	1635	CLA	CHC-C1C-C2C	-2.09	120.94	126.75
14	A6	1603	CLA	CHD-C4C-C3C	-2.09	121.80	124.88
14	B6	802	CLA	CHD-C4C-C3C	-2.09	121.80	124.88
14	B2	809	CLA	CHC-C1C-C2C	-2.09	120.94	126.75
14	B5	1830	CLA	CHD-C4C-C3C	-2.09	121.80	124.88
16	A3	856	BCR	C1-C6-C5	-2.09	119.66	122.59
14	A5	823	CLA	O2A-CGA-O1A	-2.08	118.49	123.58
14	L1	201	CLA	O2A-CGA-O1A	-2.08	118.49	123.58
14	B4	820	CLA	CHD-C4C-C3C	-2.08	121.81	124.88
14	A3	842	CLA	C12-C11-C10	-2.08	103.34	113.23
14	A3	831	CLA	O2A-CGA-O1A	-2.08	118.50	123.58
14	B1	818	CLA	CHD-C4C-C3C	-2.08	121.81	124.88
16	J4	104	BCR	C12-C13-C14	-2.08	115.75	118.94
14	B3	1815	CLA	O2A-CGA-O1A	-2.08	118.50	123.58
14	J3	101	CLA	CHD-C4C-C3C	-2.08	121.81	124.88
14	B4	836	CLA	CHD-C4C-C3C	-2.08	121.81	124.88
16	A3	852	BCR	C12-C13-C14	-2.08	115.75	118.94
14	A4	822	CLA	O2A-CGA-O1A	-2.08	118.51	123.58
14	A2	1642	CLA	O1D-CGD-CBD	-2.08	120.73	124.58
14	B2	831	CLA	O1D-CGD-CBD	-2.08	120.73	124.58
16	M4	101	BCR	C12-C13-C14	-2.08	115.75	118.94
14	B6	831	CLA	O2A-CGA-O1A	-2.08	118.51	123.58
16	A2	1650	BCR	C1-C6-C5	-2.08	119.67	122.59
16	J5	104	BCR	C24-C25-C26	-2.08	116.59	121.54
14	B3	1804	CLA	CBC-CAC-C3C	-2.08	106.64	112.42
14	A6	1623	CLA	O2A-CGA-O1A	-2.08	118.51	123.58
14	A1	805	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
16	B4	850	BCR	C23-C22-C21	-2.08	115.75	118.94
14	B1	814	CLA	CHD-C4C-C3C	-2.08	121.82	124.88
14	A4	832	CLA	C1C-C2C-C3C	-2.08	104.71	106.93
14	B4	837	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
16	J4	104	BCR	C24-C25-C26	-2.08	116.59	121.54
14	B6	838	CLA	O1D-CGD-CBD	-2.08	120.73	124.58
14	A1	822	CLA	O1D-CGD-CBD	-2.08	120.73	124.58
14	B2	811	CLA	CHD-C4C-C3C	-2.08	121.82	124.88
14	B2	816	CLA	CHD-C4C-C3C	-2.07	121.82	124.88
16	I4	101	BCR	C1-C6-C5	-2.07	119.68	122.59
14	B6	828	CLA	C4-C3-C5	-2.07	111.71	115.29
14	A3	844	CLA	CHD-C4C-C3C	-2.07	121.82	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A1	811	CLA	O2D-CGD-O1D	-2.07	119.71	123.82
14	A5	806	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
14	B1	806	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
14	A1	805	CLA	CHD-C4C-C3C	-2.07	121.82	124.88
14	B2	830	CLA	O2A-CGA-O1A	-2.07	118.53	123.58
14	A4	821	CLA	O2A-CGA-O1A	-2.07	118.53	123.58
16	M3	1602	BCR	C12-C13-C14	-2.07	115.76	118.94
14	A3	842	CLA	O2A-CGA-O1A	-2.07	118.53	123.58
14	A3	833	CLA	O1D-CGD-CBD	-2.07	120.74	124.58
14	B1	835	CLA	O2D-CGD-O1D	-2.07	119.71	123.82
14	M2	1201	CLA	CBC-CAC-C3C	-2.07	106.66	112.42
16	A4	846	BCR	C30-C25-C26	-2.07	119.68	122.59
14	A4	810	CLA	C1C-C2C-C3C	-2.07	104.72	106.93
14	B1	827	CLA	C4C-C3C-C2C	-2.07	103.83	106.90
16	F1	1302	BCR	C30-C25-C26	-2.07	119.68	122.59
14	B4	834	CLA	O1D-CGD-CBD	-2.07	120.74	124.58
14	B2	825	CLA	O2A-CGA-O1A	-2.07	118.53	123.58
16	B4	846	BCR	C23-C22-C21	-2.07	115.77	118.94
14	B5	1820	CLA	CHD-C4C-C3C	-2.07	121.83	124.88
16	A3	852	BCR	C34-C9-C10	-2.07	120.03	122.92
14	A1	820	CLA	CHD-C4C-C3C	-2.06	121.83	124.88
14	A4	802	CLA	O1D-CGD-CBD	-2.06	120.75	124.58
14	B2	809	CLA	O2A-CGA-O1A	-2.06	118.54	123.58
14	A4	804	CLA	CHD-C4C-C3C	-2.06	121.83	124.88
16	B1	849	BCR	C8-C9-C10	-2.06	115.77	118.94
14	A6	1621	CLA	CHD-C4C-C3C	-2.06	121.84	124.88
14	B5	1810	CLA	CAA-C2A-C3A	-2.06	107.15	112.81
14	A3	816	CLA	C1C-C2C-C3C	-2.06	104.72	106.93
14	B6	807	CLA	CHD-C4C-C3C	-2.06	121.84	124.88
16	A3	849	BCR	C30-C25-C26	-2.06	119.69	122.59
14	B6	812	CLA	CHD-C4C-C3C	-2.06	121.84	124.88
14	B4	843	CLA	C4C-C3C-C2C	-2.06	103.84	106.90
14	A5	804	CLA	C12-C11-C10	-2.06	106.38	113.59
14	L2	202	CLA	O2D-CGD-O1D	-2.06	119.73	123.82
14	A6	1632	CLA	O1D-CGD-CBD	-2.06	120.76	124.58
14	I6	101	CLA	O2A-CGA-O1A	-2.06	118.55	123.58
14	A1	831	CLA	CHC-C1C-C2C	-2.06	121.01	126.75
16	A3	852	BCR	C30-C25-C26	-2.06	119.70	122.59
14	A2	1635	CLA	CBC-CAC-C3C	-2.06	106.69	112.42
14	L1	206	CLA	O2A-CGA-O1A	-2.06	118.55	123.58
14	A6	1616	CLA	C1C-C2C-C3C	-2.06	104.73	106.93
14	I6	101	CLA	O1D-CGD-CBD	-2.06	120.76	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B2	801	CLA	C12-C11-C10	-2.06	103.46	113.23
14	K2	1401	CLA	O2D-CGD-O1D	-2.06	119.73	123.82
14	A1	827	CLA	C1C-C2C-C3C	-2.06	104.73	106.93
14	A2	1618	CLA	C1C-C2C-C3C	-2.06	104.73	106.93
16	A1	843	BCR	C30-C25-C26	-2.06	119.70	122.59
14	A5	822	CLA	O2A-CGA-O1A	-2.06	118.56	123.58
14	L4	201	CLA	C1C-C2C-C3C	-2.06	104.73	106.93
16	A6	1652	BCR	C33-C5-C4	-2.06	109.67	113.56
14	A6	1639	CLA	O1D-CGD-CBD	-2.06	120.77	124.58
14	B5	1810	CLA	CHC-C1C-C2C	-2.06	121.02	126.75
16	A4	849	BCR	C34-C9-C10	-2.06	120.04	122.92
16	B2	845	BCR	C38-C26-C27	-2.06	109.68	113.56
14	B1	804	CLA	C12-C11-C10	-2.05	103.48	113.23
14	A6	1606	CLA	CHD-C4C-C3C	-2.05	121.85	124.88
16	A6	1648	BCR	C12-C13-C14	-2.05	115.79	118.94
16	B4	850	BCR	C12-C13-C14	-2.05	115.79	118.94
14	B2	817	CLA	O1D-CGD-CBD	-2.05	120.77	124.58
14	B4	802	CLA	CHD-C4C-C3C	-2.05	121.85	124.88
14	B5	1803	CLA	CBC-CAC-C3C	-2.05	106.71	112.42
14	A2	1638	CLA	CHC-C1C-C2C	-2.05	121.03	126.75
14	A2	1639	CLA	CHD-C4C-C3C	-2.05	121.85	124.88
14	B4	803	CLA	C12-C11-C10	-2.05	103.50	113.23
14	L1	202	CLA	O2A-CGA-O1A	-2.05	118.57	123.58
14	B6	832	CLA	C12-C11-C10	-2.05	103.50	113.23
16	B1	849	BCR	C12-C13-C14	-2.05	115.79	118.94
14	A5	804	CLA	O2A-CGA-O1A	-2.05	118.58	123.58
14	B4	810	CLA	CHC-C1C-C2C	-2.05	121.04	126.75
14	B3	1806	CLA	CBC-CAC-C3C	-2.05	106.71	112.42
14	B4	819	CLA	O2A-CGA-O1A	-2.05	118.58	123.58
14	A4	840	CLA	C12-C11-C10	-2.05	103.51	113.23
14	K4	1401	CLA	O2D-CGD-O1D	-2.05	119.75	123.82
14	A5	839	CLA	O2A-CGA-O1A	-2.05	118.58	123.58
14	B3	1810	CLA	CHC-C1C-C2C	-2.05	121.05	126.75
14	A1	834	CLA	C1C-C2C-C3C	-2.05	104.74	106.93
14	A5	833	CLA	CHC-C1C-C2C	-2.05	121.05	126.75
16	A5	853	BCR	C23-C22-C21	-2.05	115.80	118.94
14	B3	1811	CLA	C7-C6-C5	-2.05	107.60	113.17
16	A3	856	BCR	C33-C5-C4	-2.05	109.69	113.56
14	A3	820	CLA	C1C-C2C-C3C	-2.05	104.74	106.93
16	J6	1105	BCR	C30-C25-C26	-2.05	119.71	122.59
14	A2	1632	CLA	O2A-CGA-O1A	-2.05	118.58	123.58
14	A2	1634	CLA	O1D-CGD-CBD	-2.05	120.78	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A4	806	CLA	O2D-CGD-O1D	-2.05	119.76	123.82
14	B2	801	CLA	CBC-CAC-C3C	-2.05	106.72	112.42
14	A1	836	CLA	O1D-CGD-CBD	-2.05	120.79	124.58
14	B1	802	CLA	C1C-C2C-C3C	-2.05	104.74	106.93
16	F3	201	BCR	C30-C25-C26	-2.05	119.72	122.59
14	A2	1604	CLA	C1C-C2C-C3C	-2.04	104.74	106.93
16	A6	1648	BCR	C34-C9-C10	-2.04	120.06	122.92
14	A1	819	CLA	O1D-CGD-CBD	-2.04	120.79	124.58
14	B3	1819	CLA	O2A-CGA-O1A	-2.04	118.59	123.58
16	A2	1651	BCR	C1-C6-C5	-2.04	119.72	122.59
14	B5	1832	CLA	CHD-C4C-C3C	-2.04	121.87	124.88
16	A2	1652	BCR	C30-C25-C26	-2.04	119.72	122.59
14	A1	838	CLA	C12-C11-C10	-2.04	103.55	113.23
14	A3	837	CLA	O1D-CGD-CBD	-2.04	120.80	124.58
14	A3	839	CLA	O2D-CGD-O1D	-2.04	119.77	123.82
14	B6	841	CLA	O1D-CGD-CBD	-2.04	120.80	124.58
14	A6	1633	CLA	O2A-CGA-O1A	-2.04	118.60	123.58
14	A4	822	CLA	O2D-CGD-O1D	-2.04	119.77	123.82
14	K5	102	CLA	O1D-CGD-CBD	-2.04	120.80	124.58
14	A3	820	CLA	O1D-CGD-CBD	-2.04	120.80	124.58
16	B5	1849	BCR	C15-C16-C17	-2.04	119.11	123.46
14	B2	827	CLA	O2A-CGA-O1A	-2.04	118.61	123.58
14	B1	811	CLA	C7-C6-C5	-2.04	107.62	113.17
16	B3	1849	BCR	C1-C6-C5	-2.04	119.73	122.59
16	B6	846	BCR	C38-C26-C27	-2.04	109.71	113.56
16	J3	104	BCR	C24-C25-C26	-2.04	116.68	121.54
14	B4	841	CLA	O2A-CGA-O1A	-2.04	118.61	123.58
14	M1	1201	CLA	CBC-CAC-C3C	-2.04	106.75	112.42
14	B1	810	CLA	CHC-C1C-C2C	-2.04	121.08	126.75
14	B5	1811	CLA	C7-C6-C5	-2.04	107.63	113.17
16	B1	847	BCR	C1-C6-C5	-2.04	119.73	122.59
14	B1	834	CLA	O2A-CGA-O1A	-2.04	118.61	123.58
14	A6	1641	CLA	CHD-C4C-C3C	-2.04	121.88	124.88
14	B6	840	CLA	C12-C11-C10	-2.03	103.58	113.23
14	B4	843	CLA	O1D-CGD-CBD	-2.03	120.81	124.58
14	B6	826	CLA	C4C-C3C-C2C	-2.03	103.89	106.90
14	B3	1828	CLA	O2A-CGA-O1A	-2.03	118.62	123.58
14	B2	830	CLA	O2D-CGD-O1D	-2.03	119.79	123.82
14	A4	841	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
14	A2	1622	CLA	O1D-CGD-CBD	-2.03	120.81	124.58
14	L2	205	CLA	C12-C11-C10	-2.03	103.59	113.23
14	A4	838	CLA	O2A-CGA-O1A	-2.03	118.62	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	832	CLA	C1C-C2C-C3C	-2.03	104.76	106.93
14	B6	826	CLA	C7-C6-C5	-2.03	107.65	113.17
14	L6	203	CLA	C1C-C2C-C3C	-2.03	104.76	106.93
14	L6	208	CLA	C4C-C3C-C2C	-2.03	103.89	106.90
14	B3	1833	CLA	O1D-CGD-CBD	-2.03	120.82	124.58
16	B5	1849	BCR	C1-C6-C5	-2.03	119.74	122.59
14	B6	816	CLA	O1D-CGD-CBD	-2.03	120.82	124.58
14	A4	827	CLA	C1C-C2C-C3C	-2.03	104.76	106.93
14	K6	1401	CLA	O2D-CGD-O1D	-2.03	119.80	123.82
16	L5	207	BCR	C30-C25-C26	-2.03	119.74	122.59
14	A5	841	CLA	O2A-CGA-O1A	-2.03	118.63	123.58
14	L6	207	CLA	O1D-CGD-CBD	-2.03	120.82	124.58
16	B2	846	BCR	C15-C16-C17	-2.03	119.13	123.46
14	A5	813	CLA	O2A-CGA-O1A	-2.03	118.63	123.58
14	A1	814	CLA	O2D-CGD-O1D	-2.03	119.80	123.82
14	A5	837	CLA	CHD-C4C-C3C	-2.03	121.89	124.88
16	A5	850	BCR	C1-C6-C5	-2.03	119.74	122.59
14	B4	809	CLA	O2A-CGA-O1A	-2.03	118.64	123.58
14	B5	1812	CLA	O2A-CGA-O1A	-2.03	118.64	123.58
14	L6	207	CLA	O2A-CGA-O1A	-2.03	118.64	123.58
14	J3	101	CLA	O1D-CGD-CBD	-2.03	120.82	124.58
16	B6	844	BCR	C23-C22-C21	-2.03	115.83	118.94
14	B4	828	CLA	O2A-CGA-O1A	-2.03	118.64	123.58
14	B4	807	CLA	CHC-C1C-C2C	-2.03	121.11	126.75
14	A6	1636	CLA	C1C-C2C-C3C	-2.02	104.76	106.93
14	A5	819	CLA	CHD-C4C-C3C	-2.02	121.89	124.88
14	A4	832	CLA	CHC-C1C-C2C	-2.02	121.11	126.75
14	B5	1828	CLA	C7-C6-C5	-2.02	107.67	113.17
14	A4	835	CLA	CHC-C1C-C2C	-2.02	121.11	126.75
16	B5	1850	BCR	C30-C25-C26	-2.02	119.75	122.59
14	L2	202	CLA	C1C-C2C-C3C	-2.02	104.77	106.93
14	A5	821	CLA	CHD-C4C-C3C	-2.02	121.90	124.88
16	A6	1652	BCR	C12-C13-C14	-2.02	115.84	118.94
14	A6	1615	CLA	O2D-CGD-O1D	-2.02	119.81	123.82
14	B1	805	CLA	CBC-CAC-C3C	-2.02	106.79	112.42
14	A2	1614	CLA	O2D-CGD-O1D	-2.02	119.81	123.82
14	B2	807	CLA	CHC-C1C-C2C	-2.02	121.12	126.75
14	B1	821	CLA	O1D-CGD-CBD	-2.02	120.83	124.58
14	B4	839	CLA	O2A-CGA-O1A	-2.02	118.65	123.58
14	A5	803	CLA	O2A-CGA-O1A	-2.02	118.65	123.58
14	A6	1629	CLA	C4C-C3C-C2C	-2.02	103.91	106.90
16	B6	844	BCR	C12-C13-C14	-2.02	115.84	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B2	804	CLA	CHC-C1C-C2C	-2.02	121.12	126.75
14	A4	812	CLA	O2A-CGA-O1A	-2.02	118.65	123.58
14	A4	834	CLA	O2D-CGD-O1D	-2.02	119.81	123.82
14	L4	203	CLA	C12-C11-C10	-2.02	103.65	113.23
14	B5	1828	CLA	C4C-C3C-C2C	-2.02	103.91	106.90
14	A5	818	CLA	O1D-CGD-CBD	-2.02	120.84	124.58
14	B3	1809	CLA	O2A-CGA-O1A	-2.02	118.66	123.58
14	B3	1805	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
14	A1	818	CLA	CHD-C4C-C3C	-2.02	121.90	124.88
14	B6	829	CLA	O2D-CGD-O1D	-2.02	119.82	123.82
14	B3	1810	CLA	CAA-C2A-C3A	-2.02	107.28	112.81
14	L2	206	CLA	O1D-CGD-CBD	-2.02	120.84	124.58
14	A5	816	CLA	O2A-CGA-O1A	-2.02	118.66	123.58
16	A1	847	BCR	C12-C13-C14	-2.02	115.84	118.94
14	A2	1635	CLA	C1C-C2C-C3C	-2.02	104.77	106.93
14	A2	1625	CLA	O2A-CGA-O1A	-2.02	118.66	123.58
14	A3	828	CLA	C4C-C3C-C2C	-2.02	103.91	106.90
14	A3	836	CLA	O1D-CGD-CBD	-2.02	120.84	124.58
16	B5	1846	BCR	C33-C5-C4	-2.02	109.75	113.56
16	M5	101	BCR	C12-C13-C14	-2.02	115.85	118.94
14	B1	820	CLA	C4C-C3C-C2C	-2.02	103.91	106.90
16	J4	104	BCR	C30-C25-C26	-2.02	119.76	122.59
14	A6	1606	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
14	A6	1628	CLA	C1C-C2C-C3C	-2.01	104.77	106.93
14	B3	1830	CLA	C4-C3-C5	-2.01	111.81	115.29
14	A2	1640	CLA	O1D-CGD-CBD	-2.01	120.85	124.58
14	A4	814	CLA	O2D-CGD-O1D	-2.01	119.83	123.82
14	B5	1821	CLA	C4C-C3C-C2C	-2.01	103.92	106.90
14	L6	202	CLA	O2A-CGA-O1A	-2.01	118.67	123.58
16	B2	847	BCR	C12-C13-C14	-2.01	115.85	118.94
16	F2	203	BCR	C30-C25-C26	-2.01	119.76	122.59
14	A5	828	CLA	C1C-C2C-C3C	-2.01	104.78	106.93
14	A3	823	CLA	O2A-CGA-O1A	-2.01	118.67	123.58
14	B4	821	CLA	C4C-C3C-C2C	-2.01	103.92	106.90
14	B6	808	CLA	CHC-C1C-C2C	-2.01	121.15	126.75
16	A6	1644	BCR	C38-C26-C27	-2.01	109.76	113.56
14	B6	833	CLA	O2A-CGA-O1A	-2.01	118.67	123.58
14	A5	805	CLA	C1C-C2C-C3C	-2.01	104.78	106.93
14	A4	815	CLA	C1C-C2C-C3C	-2.01	104.78	106.93
14	B1	806	CLA	C4C-C3C-C2C	-2.01	103.92	106.90
14	A1	812	CLA	CHD-C4C-C3C	-2.01	121.92	124.88
14	L1	202	CLA	C1C-C2C-C3C	-2.01	104.78	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1625	CLA	C7-C6-C5	-2.01	107.71	113.17
16	A2	1652	BCR	C1-C6-C5	-2.01	119.77	122.59
14	B5	1811	CLA	CHC-C1C-C2C	-2.01	121.16	126.75
14	A3	829	CLA	O1D-CGD-CBD	-2.01	120.86	124.58
14	A6	1605	CLA	CAA-C2A-C3A	-2.01	107.31	112.81
14	A2	1621	CLA	CHD-C4C-C3C	-2.01	121.92	124.88
16	B4	849	BCR	C1-C6-C5	-2.01	119.77	122.59
14	B4	834	CLA	O2D-CGD-O1D	-2.01	119.84	123.82
16	A4	849	BCR	C12-C13-C14	-2.01	115.86	118.94
16	I5	102	BCR	C12-C13-C14	-2.01	115.86	118.94
14	A5	833	CLA	C1C-C2C-C3C	-2.01	104.78	106.93
14	B5	1837	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
14	A1	822	CLA	CHC-C1C-C2C	-2.01	121.17	126.75
16	A2	1652	BCR	C39-C30-C25	-2.00	107.06	110.31
16	A5	853	BCR	C1-C6-C5	-2.00	119.77	122.59
14	B4	811	CLA	CHC-C1C-C2C	-2.00	121.17	126.75
14	L1	202	CLA	O2D-CGD-O1D	-2.00	119.84	123.82
14	A5	836	CLA	CHC-C1C-C2C	-2.00	121.17	126.75
14	B3	1832	CLA	CHD-C4C-C3C	-2.00	121.92	124.88
16	B1	844	BCR	C23-C22-C21	-2.00	115.87	118.94
16	J3	104	BCR	C12-C13-C14	-2.00	115.87	118.94
14	B4	807	CLA	C1C-C2C-C3C	-2.00	104.79	106.93
14	A1	804	CLA	O1D-CGD-CBD	-2.00	120.87	124.58
16	A6	1648	BCR	C30-C25-C26	-2.00	119.78	122.59
14	A5	805	CLA	CHD-C4C-C3C	-2.00	121.93	124.88
14	A4	805	CLA	CHD-C4C-C3C	-2.00	121.93	124.88
16	B1	849	BCR	C23-C22-C21	-2.00	115.87	118.94
16	B2	843	BCR	C33-C5-C4	-2.00	109.78	113.56
16	A6	1645	BCR	C30-C25-C26	-2.00	119.78	122.59
14	B1	819	CLA	C1C-C2C-C3C	-2.00	104.79	106.93
14	B3	1809	CLA	C1C-C2C-C3C	-2.00	104.79	106.93
16	I1	102	BCR	C38-C26-C27	-2.00	109.78	113.56
14	B1	827	CLA	C12-C11-C10	-2.00	103.73	113.23
16	A5	848	BCR	C1-C6-C5	-2.00	119.78	122.59
14	B2	824	CLA	C1C-C2C-C3C	-2.00	104.79	106.93
14	B4	827	CLA	CHD-C4C-C3C	-2.00	121.93	124.88
14	B2	827	CLA	C4-C3-C5	-2.00	111.84	115.29
16	B4	850	BCR	C1-C6-C5	-2.00	119.78	122.59
14	B3	1821	CLA	C4C-C3C-C2C	-2.00	103.94	106.90
14	M1	1201	CLA	CMB-C2B-C3B	2.00	128.52	124.88
14	A5	822	CLA	CMB-C2B-C3B	2.00	128.52	124.88
14	A2	1625	CLA	CAC-C3C-C4C	2.00	127.58	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1612	CLA	CAC-C3C-C4C	2.00	127.58	124.82
16	B2	842	BCR	C34-C9-C8	2.00	121.29	118.10
14	A4	821	CLA	CMC-C2C-C1C	2.00	128.12	125.05
14	B5	1834	CLA	CMB-C2B-C3B	2.00	128.52	124.88
14	A1	832	CLA	C1-C2-C3	2.00	129.64	125.96
14	B4	809	CLA	CAC-C3C-C4C	2.00	127.58	124.82
16	F1	1302	BCR	C36-C18-C19	2.00	121.29	118.10
16	A4	845	BCR	C36-C18-C19	2.00	121.29	118.10
14	B5	1834	CLA	CED-O2D-CGD	2.00	120.58	115.97
14	J6	1102	CLA	CMC-C2C-C1C	2.00	128.12	125.05
14	A5	812	CLA	C3C-C4C-NC	2.00	112.91	110.43
14	L2	206	CLA	CHB-C4A-NA	2.00	127.28	124.51
16	A1	843	BCR	C37-C22-C23	2.00	121.29	118.10
14	B5	1825	CLA	CMB-C2B-C3B	2.00	128.53	124.88
14	B2	812	CLA	CMC-C2C-C1C	2.00	128.12	125.05
16	I5	101	BCR	C37-C22-C23	2.00	121.29	118.10
14	A4	842	CLA	C4A-NA-C1A	2.00	108.91	106.32
14	A5	809	CLA	CAA-C2A-C1A	2.00	118.54	111.97
14	B6	841	CLA	CMB-C2B-C3B	2.00	128.53	124.88
14	B2	833	CLA	CAC-C3C-C4C	2.00	127.58	124.82
14	B3	1832	CLA	CMC-C2C-C1C	2.00	128.12	125.05
16	A6	1644	BCR	C33-C5-C6	2.00	126.75	124.51
14	A1	832	CLA	C4-C3-C5	2.00	118.74	115.29
14	A3	825	CLA	CAC-C3C-C4C	2.00	127.58	124.82
14	A3	805	CLA	C3B-C4B-NB	2.00	111.80	109.21
14	B3	1825	CLA	CMC-C2C-C1C	2.00	128.12	125.05
14	B2	803	CLA	CAC-C3C-C4C	2.00	127.58	124.82
14	B3	1833	CLA	CMB-C2B-C3B	2.00	128.53	124.88
14	L2	206	CLA	C3B-C4B-NB	2.00	111.80	109.21
16	L6	209	BCR	C29-C30-C25	2.00	113.61	110.48
14	B5	1837	CLA	CMC-C2C-C1C	2.00	128.12	125.05
14	A1	814	CLA	CED-O2D-CGD	2.01	120.59	115.97
14	A1	803	CLA	CMC-C2C-C1C	2.01	128.12	125.05
14	A1	822	CLA	C1-O2A-CGA	2.01	121.39	116.77
14	B2	823	CLA	CAC-C3C-C4C	2.01	127.58	124.82
14	B1	820	CLA	CAC-C3C-C4C	2.01	127.58	124.82
16	F4	203	BCR	C37-C22-C23	2.01	121.29	118.10
14	A6	1615	CLA	CED-O2D-CGD	2.01	120.59	115.97
14	A5	824	CLA	CMB-C2B-C3B	2.01	128.53	124.88
14	A2	1608	CLA	C2A-C3A-C4A	2.01	105.11	101.87
14	B4	810	CLA	CMB-C2B-C3B	2.01	128.53	124.88
14	B4	830	CLA	CMB-C2B-C3B	2.01	128.53	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	821	CLA	CMB-C2B-C3B	2.01	128.53	124.88
14	A1	801	CLA	CHB-C4A-NA	2.01	127.29	124.51
14	A1	807	CLA	CHB-C4A-NA	2.01	127.29	124.51
16	M6	1202	BCR	C36-C18-C19	2.01	121.30	118.10
14	J6	1103	CLA	CAC-C3C-C4C	2.01	127.59	124.82
14	B5	1811	CLA	CED-O2D-CGD	2.01	120.59	115.97
14	B6	836	CLA	C4A-NA-C1A	2.01	108.91	106.32
14	B1	819	CLA	C3C-C4C-NC	2.01	112.91	110.43
14	I1	101	CLA	C3B-C4B-NB	2.01	111.81	109.21
14	A1	828	CLA	CED-O2D-CGD	2.01	120.59	115.97
14	A3	806	CLA	C4-C3-C5	2.01	118.75	115.29
14	A6	1641	CLA	CAC-C3C-C4C	2.01	127.59	124.82
14	A1	824	CLA	CED-O2D-CGD	2.01	120.60	115.97
14	A1	823	CLA	CMB-C2B-C3B	2.01	128.54	124.88
14	B6	817	CLA	CMB-C2B-C3B	2.01	128.54	124.88
14	A4	840	CLA	CAC-C3C-C4C	2.01	127.59	124.82
14	B5	1802	CLA	O2D-CGD-CBD	2.01	114.84	111.28
14	B5	1840	CLA	CMC-C2C-C1C	2.01	128.13	125.05
14	A6	1617	CLA	CMB-C2B-C3B	2.01	128.54	124.88
14	A2	1616	CLA	CMB-C2B-C3B	2.01	128.54	124.88
14	B6	833	CLA	C4A-NA-C1A	2.01	108.91	106.32
16	F4	201	BCR	C37-C22-C23	2.01	121.30	118.10
14	B2	824	CLA	C3B-C4B-NB	2.01	111.81	109.21
14	A5	818	CLA	CMB-C2B-C3B	2.01	128.54	124.88
14	A6	1638	CLA	CMC-C2C-C1C	2.01	128.13	125.05
16	F2	203	BCR	C40-C30-C25	2.01	113.57	110.31
16	B4	847	BCR	C35-C13-C12	2.01	121.30	118.10
16	B2	846	BCR	C29-C30-C25	2.01	113.62	110.48
16	L6	204	BCR	C32-C1-C6	2.01	113.57	110.31
14	A3	835	CLA	C4A-NA-C1A	2.01	108.92	106.32
14	B4	830	CLA	CBA-CAA-C2A	2.01	119.78	113.82
14	B3	1832	CLA	C3C-C4C-NC	2.01	112.92	110.43
14	A4	817	CLA	CMC-C2C-C1C	2.01	128.13	125.05
14	A4	815	CLA	CAC-C3C-C4C	2.01	127.59	124.82
14	A4	807	CLA	CHB-C4A-NA	2.01	127.29	124.51
14	J5	102	CLA	CAC-C3C-C4C	2.01	127.59	124.82
14	A1	828	CLA	CMD-C2D-C3D	2.01	128.54	124.88
14	A4	814	CLA	CED-O2D-CGD	2.01	120.60	115.97
14	A4	809	CLA	CMC-C2C-C1C	2.01	128.13	125.05
16	J3	104	BCR	C34-C9-C8	2.01	121.30	118.10
14	B1	840	CLA	CED-O2D-CGD	2.01	120.61	115.97
14	B3	1807	CLA	CED-O2D-CGD	2.01	120.61	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L3	203	CLA	CMB-C2B-C3B	2.01	128.54	124.88
16	L1	203	BCR	C38-C26-C25	2.01	126.76	124.51
16	B4	846	BCR	C1-C6-C7	2.01	121.39	115.73
14	A1	828	CLA	CMC-C2C-C1C	2.01	128.13	125.05
16	B3	1849	BCR	C30-C25-C24	2.01	121.39	115.73
16	B1	848	BCR	C37-C22-C23	2.01	121.31	118.10
14	A2	1642	CLA	C4-C3-C5	2.01	118.35	115.96
14	L1	202	CLA	CED-O2D-CGD	2.01	120.61	115.97
14	A3	811	CLA	CMB-C2B-C3B	2.01	128.55	124.88
14	A6	1620	CLA	C1-O2A-CGA	2.01	121.41	116.77
14	A4	837	CLA	CAC-C3C-C4C	2.01	127.60	124.82
14	A2	1617	CLA	CAC-C3C-C4C	2.01	127.60	124.82
14	A3	820	CLA	C3C-C4C-NC	2.01	112.92	110.43
14	A2	1640	CLA	CMC-C2C-C1C	2.01	128.14	125.05
14	A1	817	CLA	CMB-C2B-C3B	2.01	128.55	124.88
14	B3	1827	CLA	O2A-CGA-CBA	2.01	120.41	112.32
14	J4	102	CLA	CMC-C2C-C1C	2.02	128.14	125.05
14	L6	202	CLA	C1-C2-C3	2.02	129.67	125.96
14	A5	802	CLA	CMC-C2C-C1C	2.02	128.14	125.05
14	B6	838	CLA	C3C-C4C-NC	2.02	112.93	110.43
16	M4	101	BCR	C36-C18-C19	2.02	121.31	118.10
16	A6	1652	BCR	C38-C26-C25	2.02	126.77	124.51
14	B1	833	CLA	CMB-C2B-C3B	2.02	128.55	124.88
16	B3	1847	BCR	C28-C27-C26	2.02	117.53	113.99
14	A3	808	CLA	CHB-C4A-NA	2.02	127.30	124.51
14	A3	838	CLA	CMC-C2C-C1C	2.02	128.14	125.05
14	B5	1841	CLA	CAC-C3C-C4C	2.02	127.60	124.82
14	A3	823	CLA	C1-O2A-CGA	2.02	121.42	116.77
16	J6	1105	BCR	C33-C5-C6	2.02	126.77	124.51
14	A1	822	CLA	CED-O2D-CGD	2.02	120.62	115.97
14	B4	831	CLA	CAC-C3C-C4C	2.02	127.60	124.82
16	I3	101	BCR	C37-C22-C23	2.02	121.31	118.10
16	L2	201	BCR	C37-C22-C23	2.02	121.31	118.10
14	A4	812	CLA	C3B-C4B-NB	2.02	111.82	109.21
14	A2	1615	CLA	C3B-C4B-NB	2.02	111.82	109.21
14	A1	838	CLA	C11-C10-C8	2.02	122.36	115.73
14	B5	1819	CLA	CAC-C3C-C4C	2.02	127.60	124.82
14	A6	1604	CLA	CAC-C3C-C4C	2.02	127.60	124.82
14	A5	831	CLA	C3C-C4C-NC	2.02	112.93	110.43
14	A5	806	CLA	C2A-C3A-C4A	2.02	105.13	101.87
14	B4	840	CLA	CMC-C2C-C1C	2.02	128.15	125.05
14	K5	102	CLA	CMC-C2C-C1C	2.02	128.15	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F5	1302	BCR	C37-C22-C23	2.02	121.32	118.10
14	A3	841	CLA	CED-O2D-CGD	2.02	120.63	115.97
14	J2	101	CLA	CMB-C2B-C3B	2.02	128.56	124.88
14	A3	817	CLA	CMB-C2B-C3B	2.02	128.56	124.88
14	B4	810	CLA	C3B-C4B-NB	2.02	111.82	109.21
14	B5	1805	CLA	C11-C10-C8	2.02	122.37	115.73
16	B2	846	BCR	C34-C9-C8	2.02	121.32	118.10
14	B6	824	CLA	C6-C5-C3	2.02	117.72	112.82
14	B2	838	CLA	CMB-C2B-C3B	2.02	128.56	124.88
14	B1	838	CLA	C1-C2-C3	2.02	129.68	125.96
14	A4	813	CLA	CMB-C2B-C3B	2.02	128.56	124.88
16	B6	844	BCR	C33-C5-C6	2.02	126.77	124.51
16	I5	102	BCR	C32-C1-C6	2.02	113.59	110.31
14	B3	1805	CLA	CHB-C4A-NA	2.02	127.31	124.51
14	A1	810	CLA	C3B-C4B-NB	2.02	111.83	109.21
14	A2	1601	CLA	CMC-C2C-C1C	2.02	128.15	125.05
14	J6	1101	CLA	CMB-C2B-C3B	2.02	128.56	124.88
14	A2	1624	CLA	C3C-C4C-NC	2.02	112.94	110.43
14	B5	1828	CLA	C4A-NA-C1A	2.02	108.93	106.32
16	B5	1849	BCR	C30-C25-C24	2.02	121.42	115.73
14	B6	804	CLA	CMC-C2C-C1C	2.02	128.15	125.05
14	A6	1613	CLA	C4A-NA-C1A	2.02	108.93	106.32
16	A4	848	BCR	C34-C9-C8	2.02	121.33	118.10
14	B5	1820	CLA	CMC-C2C-C1C	2.03	128.15	125.05
14	A1	829	CLA	CMC-C2C-C1C	2.03	128.15	125.05
14	J4	101	CLA	CMB-C2B-C3B	2.03	128.57	124.88
14	A2	1645	CLA	CAC-C3C-C4C	2.03	127.61	124.82
16	B1	848	BCR	C32-C1-C6	2.03	113.59	110.31
14	A3	835	CLA	C4-C3-C5	2.03	118.78	115.29
14	A3	818	CLA	CMC-C2C-C1C	2.03	128.15	125.05
16	F2	201	BCR	C37-C22-C23	2.03	121.33	118.10
14	A1	828	CLA	CAC-C3C-C4C	2.03	127.61	124.82
14	A2	1608	CLA	C3B-C4B-NB	2.03	111.83	109.21
14	B5	1838	CLA	CMC-C2C-C1C	2.03	128.16	125.05
14	A6	1636	CLA	C1-O2A-CGA	2.03	121.44	116.77
14	A5	836	CLA	CAC-C3C-C4C	2.03	127.61	124.82
14	B3	1821	CLA	CAC-C3C-C4C	2.03	127.61	124.82
14	A6	1611	CLA	C3B-C4B-NB	2.03	111.83	109.21
14	B3	1818	CLA	CAC-C3C-C4C	2.03	127.62	124.82
14	A4	819	CLA	C3C-C4C-NC	2.03	112.94	110.43
14	B5	1806	CLA	C3B-C4B-NB	2.03	111.83	109.21
14	B1	815	CLA	C1-C2-C3	2.03	129.69	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B2	844	BCR	C34-C9-C8	2.03	121.33	118.10
14	K5	102	CLA	CED-O2D-CGD	2.03	120.64	115.97
14	L6	206	CLA	CMB-C2B-C3B	2.03	128.57	124.88
14	B6	822	CLA	C10-C8-C9	2.03	120.11	110.48
14	B1	853	CLA	C1-O2A-CGA	2.03	121.44	116.77
14	A5	843	CLA	C1-O2A-CGA	2.03	121.44	116.77
14	A1	821	CLA	C4A-NA-C1A	2.03	108.94	106.32
14	B2	809	CLA	CMC-C2C-C1C	2.03	128.16	125.05
14	B1	814	CLA	C3B-C4B-NB	2.03	111.83	109.21
14	A4	829	CLA	CMC-C2C-C1C	2.03	128.16	125.05
14	B6	805	CLA	CAC-C3C-C4C	2.03	127.62	124.82
14	A5	836	CLA	C4A-NA-C1A	2.03	108.94	106.32
14	A3	802	CLA	CMC-C2C-C1C	2.03	128.16	125.05
14	B6	824	CLA	CAC-C3C-C4C	2.03	127.62	124.82
14	B3	1801	CLA	C1-C2-C3	2.03	129.70	125.96
14	L1	207	CLA	CMB-C2B-C3B	2.03	128.58	124.88
14	A1	810	CLA	C4A-NA-C1A	2.03	108.94	106.32
14	K4	1401	CLA	CED-O2D-CGD	2.03	120.65	115.97
16	F6	203	BCR	C37-C22-C23	2.03	121.33	118.10
14	A2	1627	CLA	CAC-C3C-C4C	2.03	127.62	124.82
14	A3	816	CLA	CAC-C3C-C4C	2.03	127.62	124.82
16	B4	848	BCR	C35-C13-C12	2.03	119.17	114.59
14	B3	1835	CLA	C4A-NA-C1A	2.03	108.94	106.32
14	B3	1806	CLA	C4A-NA-C1A	2.03	108.94	106.32
14	A5	810	CLA	CMB-C2B-C3B	2.03	128.58	124.88
14	B6	812	CLA	CMB-C2B-C3B	2.03	128.58	124.88
14	A1	820	CLA	CAC-C3C-C4C	2.03	127.62	124.82
14	A3	826	CLA	CED-O2D-CGD	2.03	120.65	115.97
14	A1	831	CLA	CMB-C2B-C3B	2.03	128.58	124.88
14	A2	1611	CLA	CAA-C2A-C1A	2.03	118.64	111.97
14	B3	1810	CLA	CAC-C3C-C4C	2.03	127.62	124.82
14	B3	1822	CLA	C3C-C4C-NC	2.03	112.95	110.43
14	B2	837	CLA	C3C-C4C-NC	2.03	112.95	110.43
14	B1	837	CLA	CMC-C2C-C1C	2.03	128.17	125.05
14	A5	834	CLA	C4-C3-C5	2.03	118.80	115.29
14	B4	828	CLA	C4A-NA-C1A	2.03	108.95	106.32
16	B5	1850	BCR	C37-C22-C23	2.03	121.34	118.10
14	B5	1807	CLA	CED-O2D-CGD	2.03	120.66	115.97
14	A4	808	CLA	CAA-C2A-C1A	2.03	118.64	111.97
14	A2	1631	CLA	CMD-C2D-C3D	2.03	128.59	124.88
14	A5	833	CLA	CED-O2D-CGD	2.04	120.66	115.97
14	A1	834	CLA	C1-O2A-CGA	2.04	121.46	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B1	846	BCR	C35-C13-C12	2.04	119.18	114.59
16	B4	845	BCR	C34-C9-C8	2.04	121.34	118.10
16	A2	1650	BCR	C36-C18-C19	2.04	121.34	118.10
14	B2	803	CLA	CHB-C4A-NA	2.04	127.33	124.51
14	A6	1638	CLA	CAC-C3C-C4C	2.04	127.63	124.82
14	A5	806	CLA	CAA-CBA-CGA	2.04	119.43	113.35
14	B6	838	CLA	CHB-C4A-NA	2.04	127.33	124.51
14	A3	815	CLA	CED-O2D-CGD	2.04	120.66	115.97
14	B6	839	CLA	CMC-C2C-C1C	2.04	128.17	125.05
14	F2	204	CLA	CMC-C2C-C1C	2.04	128.17	125.05
14	A1	815	CLA	CAC-C3C-C4C	2.04	127.63	124.82
14	B1	827	CLA	C3B-C4B-NB	2.04	111.84	109.21
16	F2	203	BCR	C37-C22-C23	2.04	121.34	118.10
14	A3	822	CLA	CMB-C2B-C3B	2.04	128.59	124.88
16	M3	1602	BCR	C36-C18-C19	2.04	121.34	118.10
16	M5	101	BCR	C40-C30-C25	2.04	113.61	110.31
14	A6	1603	CLA	O2D-CGD-CBD	2.04	114.90	111.28
14	B5	1826	CLA	CMC-C2C-C1C	2.04	128.17	125.05
14	B1	801	CLA	CMC-C2C-C1C	2.04	128.17	125.05
14	A4	809	CLA	CMB-C2B-C3B	2.04	128.59	124.88
14	B2	840	CLA	CMB-C2B-C3B	2.04	128.59	124.88
14	A3	826	CLA	CHB-C4A-NA	2.04	127.33	124.51
14	B1	804	CLA	CHB-C4A-NA	2.04	127.33	124.51
14	B3	1838	CLA	CED-O2D-CGD	2.04	120.67	115.97
14	A4	803	CLA	CAC-C3C-C4C	2.04	127.63	124.82
14	A3	815	CLA	C3B-C4B-NB	2.04	111.85	109.21
14	B4	841	CLA	CMB-C2B-C3B	2.04	128.59	124.88
14	M2	1201	CLA	CMB-C2B-C3B	2.04	128.59	124.88
14	A4	825	CLA	CHB-C4A-NA	2.04	127.33	124.51
14	A5	820	CLA	C3C-C4C-NC	2.04	112.95	110.43
16	J6	1105	BCR	C37-C22-C23	2.04	121.35	118.10
16	J1	104	BCR	C37-C22-C23	2.04	121.35	118.10
14	B1	854	CLA	C4A-NA-C1A	2.04	108.95	106.32
16	I5	101	BCR	C34-C9-C8	2.04	121.35	118.10
16	A1	843	BCR	C33-C5-C6	2.04	126.79	124.51
14	B1	839	CLA	CHB-C4A-NA	2.04	127.33	124.51
14	A2	1639	CLA	CAC-C3C-C4C	2.04	127.63	124.82
14	A1	802	CLA	C3C-C4C-NC	2.04	112.96	110.43
14	J5	101	CLA	CMB-C2B-C3B	2.04	128.60	124.88
14	B1	818	CLA	CAC-C3C-C4C	2.04	127.64	124.82
14	A6	1635	CLA	C4A-NA-C1A	2.04	108.96	106.32
14	B6	837	CLA	CED-O2D-CGD	2.04	120.67	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1622	CLA	CMC-C2C-C1C	2.04	128.18	125.05
14	A5	841	CLA	CAC-C3C-C4C	2.04	127.64	124.82
16	L3	201	BCR	C37-C22-C23	2.04	121.35	118.10
14	A2	1630	CLA	CED-O2D-CGD	2.04	120.68	115.97
16	B4	848	BCR	C38-C26-C25	2.04	126.80	124.51
14	A4	842	CLA	CAC-C3C-C4C	2.04	127.64	124.82
14	A6	1624	CLA	CMB-C2B-C3B	2.04	128.60	124.88
14	B6	829	CLA	CAC-C3C-C4C	2.04	127.64	124.82
16	F5	1302	BCR	C36-C18-C19	2.04	121.36	118.10
16	B5	1849	BCR	C34-C9-C8	2.04	121.36	118.10
14	A6	1637	CLA	CMC-C2C-C1C	2.04	128.18	125.05
16	B1	843	BCR	C34-C9-C8	2.05	121.36	118.10
14	B5	1838	CLA	C4A-NA-C1A	2.05	108.96	106.32
14	A3	827	CLA	CAC-C3C-C4C	2.05	127.64	124.82
14	B1	836	CLA	CMC-C2C-C1C	2.05	128.18	125.05
14	B6	830	CLA	C4A-NA-C1A	2.05	108.96	106.32
14	B1	807	CLA	CED-O2D-CGD	2.05	120.68	115.97
14	B4	821	CLA	CAC-C3C-C4C	2.05	127.64	124.82
14	A3	818	CLA	CMB-C2B-C3B	2.05	128.61	124.88
14	A1	808	CLA	CMC-C2C-C1C	2.05	128.19	125.05
14	B5	1816	CLA	C1-C2-C3	2.05	129.73	125.96
14	B4	835	CLA	C4A-NA-C1A	2.05	108.96	106.32
14	B3	1805	CLA	C11-C10-C8	2.05	122.45	115.73
14	A2	1636	CLA	C4-C3-C5	2.05	118.82	115.29
14	A4	836	CLA	CAC-C3C-C4C	2.05	127.64	124.82
14	F2	204	CLA	CAC-C3C-C4C	2.05	127.64	124.82
14	B3	1837	CLA	CMC-C2C-C1C	2.05	128.19	125.05
16	I5	102	BCR	C38-C26-C25	2.05	126.80	124.51
14	A5	828	CLA	CED-O2D-CGD	2.05	120.69	115.97
14	A3	823	CLA	CED-O2D-CGD	2.05	120.69	115.97
14	B4	833	CLA	CMB-C2B-C3B	2.05	128.61	124.88
16	A6	1646	BCR	C36-C18-C19	2.05	121.36	118.10
14	A4	811	CLA	CAC-C3C-C4C	2.05	127.64	124.82
14	B5	1826	CLA	C6-C5-C3	2.05	117.78	112.82
14	B1	820	CLA	CMB-C2B-C3B	2.05	128.61	124.88
16	M4	101	BCR	C35-C13-C12	2.05	121.36	118.10
16	J2	103	BCR	C37-C22-C23	2.05	121.36	118.10
14	J4	101	CLA	CAC-C3C-C4C	2.05	127.65	124.82
14	B5	1812	CLA	C4A-NA-C1A	2.05	108.97	106.32
16	B4	848	BCR	C36-C18-C19	2.05	121.36	118.10
14	L2	202	CLA	CMC-C2C-C1C	2.05	128.19	125.05
14	B4	835	CLA	CED-O2D-CGD	2.05	120.69	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B3	1838	CLA	CAC-C3C-C4C	2.05	127.65	124.82
16	L4	208	BCR	C37-C22-C23	2.05	121.37	118.10
16	A1	846	BCR	C34-C9-C8	2.05	121.37	118.10
14	A3	814	CLA	CMB-C2B-C3B	2.05	128.61	124.88
14	B1	810	CLA	CHB-C4A-NA	2.05	127.35	124.51
16	B6	847	BCR	C30-C25-C24	2.05	121.49	115.73
14	B4	816	CLA	C1-C2-C3	2.05	129.74	125.96
14	B2	823	CLA	C6-C5-C3	2.05	117.79	112.82
14	B6	835	CLA	CMC-C2C-C1C	2.05	128.19	125.05
14	K6	1401	CLA	CMC-C2C-C1C	2.05	128.19	125.05
14	B4	812	CLA	C4A-NA-C1A	2.05	108.97	106.32
14	A3	822	CLA	CMC-C2C-C1C	2.05	128.19	125.05
14	A6	1622	CLA	CMB-C2B-C3B	2.05	128.62	124.88
14	B4	812	CLA	CAC-C3C-C4C	2.05	127.65	124.82
16	F3	203	BCR	C37-C22-C23	2.05	121.37	118.10
16	B2	846	BCR	C30-C25-C24	2.05	121.50	115.73
16	J5	104	BCR	C37-C22-C23	2.05	121.37	118.10
14	J4	102	CLA	CAC-C3C-C4C	2.05	127.65	124.82
14	A2	1609	CLA	CMC-C2C-C1C	2.05	128.20	125.05
14	A2	1602	CLA	CHB-C4A-NA	2.05	127.35	124.51
16	B1	845	BCR	C34-C9-C8	2.05	121.37	118.10
16	B1	844	BCR	C1-C6-C7	2.05	121.50	115.73
14	A2	1619	CLA	CMB-C2B-C3B	2.06	128.62	124.88
14	A6	1613	CLA	C3B-C4B-NB	2.06	111.87	109.21
14	B5	1822	CLA	CHB-C4A-NA	2.06	127.35	124.51
14	A2	1639	CLA	CMC-C2C-C1C	2.06	128.20	125.05
14	A2	1612	CLA	CMB-C2B-C3B	2.06	128.62	124.88
14	B4	814	CLA	CMC-C2C-C1C	2.06	128.20	125.05
16	B2	845	BCR	C35-C13-C12	2.06	119.23	114.59
14	B5	1841	CLA	CED-O2D-CGD	2.06	120.71	115.97
14	A3	831	CLA	C3C-C4C-NC	2.06	112.97	110.43
14	L3	204	CLA	C3C-C4C-NC	2.06	112.97	110.43
16	A6	1646	BCR	C38-C26-C25	2.06	126.81	124.51
14	A2	1620	CLA	CMB-C2B-C3B	2.06	128.62	124.88
14	A1	812	CLA	C4A-NA-C1A	2.06	108.98	106.32
14	B2	835	CLA	C4A-NA-C1A	2.06	108.98	106.32
14	K2	1401	CLA	CAC-C3C-C4C	2.06	127.66	124.82
16	F5	1302	BCR	C40-C30-C25	2.06	113.64	110.31
16	B2	844	BCR	C40-C30-C25	2.06	113.65	110.31
16	A2	1649	BCR	C36-C18-C19	2.06	121.38	118.10
14	A2	1612	CLA	CMC-C2C-C1C	2.06	128.21	125.05
16	B2	844	BCR	C35-C13-C12	2.06	121.38	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	809	CLA	C3C-C4C-NC	2.06	112.98	110.43
14	A5	830	CLA	CMC-C2C-C1C	2.06	128.21	125.05
14	A1	830	CLA	CMC-C2C-C1C	2.06	128.21	125.05
14	A2	1606	CLA	CAC-C3C-C4C	2.06	127.66	124.82
14	B5	1824	CLA	CAC-C3C-C4C	2.06	127.66	124.82
14	A5	842	CLA	CED-O2D-CGD	2.06	120.72	115.97
14	B6	804	CLA	CHB-C4A-NA	2.06	127.36	124.51
16	B5	1846	BCR	C1-C6-C7	2.06	121.52	115.73
14	B1	837	CLA	C4A-NA-C1A	2.06	108.98	106.32
16	L6	204	BCR	C38-C26-C25	2.06	126.82	124.51
14	B6	809	CLA	C3B-C4B-NB	2.06	111.88	109.21
14	B6	802	CLA	CMB-C2B-C3B	2.06	128.63	124.88
14	A5	820	CLA	C1-O2A-CGA	2.06	121.52	116.77
14	B4	842	CLA	C11-C10-C8	2.06	122.50	115.73
14	A1	805	CLA	C3B-C4B-NB	2.06	111.88	109.21
16	B4	847	BCR	C34-C9-C8	2.06	121.39	118.10
19	B4	851	LMG	O7-C10-C11	2.06	115.90	111.55
16	B1	847	BCR	C30-C25-C24	2.06	121.53	115.73
14	A3	810	CLA	CMC-C2C-C1C	2.06	128.21	125.05
14	B6	839	CLA	CMB-C2B-C3B	2.06	128.64	124.88
14	A6	1637	CLA	CAC-C3C-C4C	2.06	127.67	124.82
14	L6	207	CLA	CAC-C3C-C4C	2.06	127.67	124.82
14	B5	1818	CLA	C4-C3-C5	2.06	118.85	115.29
14	B3	1840	CLA	C3C-C4C-NC	2.06	112.98	110.43
14	A2	1638	CLA	CMC-C2C-C1C	2.06	128.21	125.05
14	B6	812	CLA	CMC-C2C-C1C	2.06	128.21	125.05
14	A3	801	CLA	CGD-CBD-CAD	2.07	117.42	110.73
14	B6	826	CLA	C3B-C4B-NB	2.07	111.88	109.21
14	B6	838	CLA	C4A-NA-C1A	2.07	108.99	106.32
14	A6	1634	CLA	C4-C3-C5	2.07	118.85	115.29
14	A3	812	CLA	CAC-C3C-C4C	2.07	127.67	124.82
16	A1	844	BCR	C36-C18-C19	2.07	121.39	118.10
14	B4	826	CLA	C6-C5-C3	2.07	117.83	112.82
14	B3	1842	CLA	C3B-C4B-NB	2.07	111.88	109.21
14	A2	1643	CLA	C6-C5-C3	2.07	117.83	112.82
16	B4	849	BCR	C37-C22-C23	2.07	121.39	118.10
14	B4	806	CLA	C4A-NA-C1A	2.07	108.99	106.32
14	A1	835	CLA	C3C-C4C-NC	2.07	112.99	110.43
14	A3	844	CLA	CAC-C3C-C4C	2.07	127.67	124.82
14	A6	1626	CLA	CHB-C4A-NA	2.07	127.37	124.51
14	B2	821	CLA	C3B-C4B-NB	2.07	111.88	109.21
16	F1	1302	BCR	C37-C22-C23	2.07	121.39	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	838	CLA	C3C-C4C-NC	2.07	112.99	110.43
14	A2	1605	CLA	CMC-C2C-C1C	2.07	128.22	125.05
14	A2	1642	CLA	C3B-C4B-NB	2.07	111.88	109.21
14	A3	836	CLA	CMB-C2B-C3B	2.07	128.65	124.88
14	B2	838	CLA	CMC-C2C-C1C	2.07	128.22	125.05
14	B1	809	CLA	CED-O2D-CGD	2.07	120.74	115.97
14	B1	826	CLA	C3B-C4B-NB	2.07	111.89	109.21
14	A3	842	CLA	CED-O2D-CGD	2.07	120.74	115.97
16	B4	846	BCR	C35-C13-C12	2.07	121.40	118.10
14	A1	832	CLA	CMB-C2B-C3B	2.07	128.65	124.88
16	B3	1846	BCR	C37-C22-C23	2.07	121.40	118.10
14	A4	817	CLA	CMB-C2B-C3B	2.07	128.65	124.88
14	A3	813	CLA	C3B-C4B-NB	2.07	111.89	109.21
14	A4	808	CLA	C4A-NA-C1A	2.07	108.99	106.32
14	B6	824	CLA	CED-O2D-CGD	2.07	120.74	115.97
16	B1	844	BCR	C37-C22-C23	2.07	121.40	118.10
14	B3	1816	CLA	C1-C2-C3	2.07	129.77	125.96
14	A6	1634	CLA	CMB-C2B-C3B	2.07	128.65	124.88
14	K6	1401	CLA	CED-O2D-CGD	2.07	120.74	115.97
14	B6	828	CLA	C5-C3-C2	2.07	125.31	121.10
14	B6	817	CLA	CAC-C3C-C4C	2.07	127.68	124.82
14	A5	806	CLA	C3B-C4B-NB	2.07	111.89	109.21
14	A3	806	CLA	C3B-C4B-NB	2.07	111.89	109.21
16	A2	1652	BCR	C34-C9-C8	2.07	121.40	118.10
14	A3	836	CLA	C4A-NA-C1A	2.07	108.99	106.32
14	B3	1835	CLA	CED-O2D-CGD	2.07	120.74	115.97
14	A3	845	CLA	CED-O2D-CGD	2.07	120.74	115.97
16	A4	847	BCR	C36-C18-C19	2.07	121.40	118.10
14	J1	102	CLA	CMC-C2C-C1C	2.07	128.22	125.05
14	A6	1610	CLA	CMB-C2B-C3B	2.07	128.65	124.88
14	B3	1826	CLA	C6-C5-C3	2.07	117.84	112.82
16	B5	1848	BCR	C35-C13-C12	2.07	119.27	114.59
14	B5	1821	CLA	CAC-C3C-C4C	2.07	127.68	124.82
14	A5	833	CLA	CMB-C2B-C3B	2.07	128.66	124.88
16	B1	847	BCR	C34-C9-C8	2.07	121.40	118.10
16	B6	844	BCR	C1-C6-C7	2.07	121.56	115.73
14	A5	813	CLA	C4A-NA-C1A	2.07	109.00	106.32
14	J3	102	CLA	CAC-C3C-C4C	2.08	127.68	124.82
14	B5	1809	CLA	CAC-C3C-C4C	2.08	127.68	124.82
14	B6	826	CLA	CAC-C3C-C4C	2.08	127.68	124.82
14	A2	1631	CLA	C3B-C4B-NB	2.08	111.89	109.21
14	A4	804	CLA	C3B-C4B-NB	2.08	111.89	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1810	CLA	CHB-C4A-NA	2.08	127.38	124.51
14	A1	809	CLA	CMC-C2C-C1C	2.08	128.23	125.05
14	A6	1633	CLA	CMC-C2C-C1C	2.08	128.23	125.05
16	B5	1845	BCR	C34-C9-C8	2.08	121.41	118.10
14	A6	1637	CLA	C3C-C4C-NC	2.08	113.00	110.43
14	B1	825	CLA	C6-C5-C3	2.08	117.85	112.82
14	B3	1814	CLA	CMB-C2B-C3B	2.08	128.66	124.88
14	J3	102	CLA	CMC-C2C-C1C	2.08	128.23	125.05
14	B6	808	CLA	C3B-C4B-NB	2.08	111.90	109.21
14	A1	803	CLA	CAC-C3C-C4C	2.08	127.69	124.82
14	A3	818	CLA	CAC-C3C-C4C	2.08	127.69	124.82
14	A2	1611	CLA	C4A-NA-C1A	2.08	109.00	106.32
14	J5	102	CLA	CMC-C2C-C1C	2.08	128.24	125.05
16	B1	845	BCR	C35-C13-C12	2.08	121.41	118.10
14	B3	1803	CLA	CHB-C4A-NA	2.08	127.39	124.51
14	B6	834	CLA	CAC-C3C-C4C	2.08	127.69	124.82
16	F6	203	BCR	C40-C30-C25	2.08	113.68	110.31
16	F3	203	BCR	C40-C30-C25	2.08	113.68	110.31
14	B5	1803	CLA	CMC-C2C-C1C	2.08	128.24	125.05
14	X3	102	CLA	C4A-NA-C1A	2.08	109.01	106.32
14	F5	1301	CLA	CAC-C3C-C4C	2.08	127.69	124.82
16	B3	1848	BCR	C36-C18-C19	2.08	121.41	118.10
14	A3	802	CLA	CMB-C2B-C3B	2.08	128.67	124.88
14	B6	806	CLA	CED-O2D-CGD	2.08	120.77	115.97
14	B2	802	CLA	C9-C8-C10	2.08	118.93	111.36
14	A1	827	CLA	CED-O2D-CGD	2.08	120.77	115.97
14	X2	1701	CLA	CMB-C2B-C3B	2.08	128.67	124.88
14	A6	1631	CLA	C2C-C1C-NC	2.08	112.25	110.09
14	A1	811	CLA	C3C-C4C-NC	2.08	113.01	110.43
14	A2	1615	CLA	C4A-NA-C1A	2.08	109.01	106.32
16	A5	848	BCR	C38-C26-C25	2.08	126.84	124.51
16	B3	1849	BCR	C37-C22-C23	2.08	121.42	118.10
14	A2	1642	CLA	CMC-C2C-C1C	2.08	128.24	125.05
14	A1	808	CLA	CAA-C2A-C1A	2.08	118.80	111.97
14	B3	1838	CLA	CMC-C2C-C1C	2.08	128.24	125.05
14	B4	837	CLA	CMC-C2C-C1C	2.08	128.24	125.05
14	B5	1829	CLA	CED-O2D-CGD	2.08	120.77	115.97
16	B1	845	BCR	C28-C27-C26	2.08	117.65	113.99
14	A1	838	CLA	CAC-C3C-C4C	2.08	127.69	124.82
14	A2	1636	CLA	C1-C2-C3	2.08	129.80	125.96
16	J5	105	BCR	C37-C22-C23	2.09	121.42	118.10
14	A2	1606	CLA	CMC-C2C-C1C	2.09	128.25	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1838	CLA	CED-O2D-CGD	2.09	120.78	115.97
14	B3	1810	CLA	CHB-C4A-NA	2.09	127.40	124.51
14	B4	805	CLA	CHB-C4A-NA	2.09	127.40	124.51
14	A5	816	CLA	CAC-C3C-C4C	2.09	127.70	124.82
14	B4	827	CLA	C4A-NA-C1A	2.09	109.01	106.32
16	A3	851	BCR	C34-C9-C8	2.09	121.42	118.10
14	A3	809	CLA	CAA-C2A-C1A	2.09	118.81	111.97
14	B2	823	CLA	CMC-C2C-C1C	2.09	128.25	125.05
14	A1	805	CLA	CAA-CBA-CGA	2.09	119.58	113.35
16	L6	204	BCR	C2-C1-C6	2.09	113.74	110.48
14	A2	1643	CLA	C11-C10-C8	2.09	122.59	115.73
14	J6	1102	CLA	C4A-NA-C1A	2.09	109.02	106.32
14	B1	853	CLA	CMC-C2C-C1C	2.09	128.25	125.05
16	M4	101	BCR	C32-C1-C6	2.09	113.69	110.31
14	A5	822	CLA	C4A-NA-C1A	2.09	109.02	106.32
14	B4	831	CLA	CMC-C2C-C1C	2.09	128.25	125.05
14	A1	830	CLA	C2C-C1C-NC	2.09	112.25	110.09
14	B6	819	CLA	CAC-C3C-C4C	2.09	127.70	124.82
16	B3	1847	BCR	C35-C13-C12	2.09	121.43	118.10
14	J6	1102	CLA	CMB-C2B-C3B	2.09	128.69	124.88
14	B5	1843	CLA	CMB-C2B-C3B	2.09	128.69	124.88
19	B6	848	LMG	O7-C10-C11	2.09	115.95	111.55
14	J2	101	CLA	C4A-NA-C1A	2.09	109.02	106.32
14	A5	831	CLA	C2C-C1C-NC	2.09	112.25	110.09
14	A3	825	CLA	CED-O2D-CGD	2.09	120.79	115.97
14	K3	1401	CLA	CED-O2D-CGD	2.09	120.79	115.97
14	B1	854	CLA	CAA-C2A-C1A	2.09	118.83	111.97
14	A6	1606	CLA	C3B-C4B-NB	2.09	111.91	109.21
14	A2	1614	CLA	CAC-C3C-C4C	2.09	127.70	124.82
14	B2	809	CLA	CAA-C2A-C1A	2.09	118.83	111.97
14	A1	837	CLA	CMC-C2C-C1C	2.09	128.25	125.05
14	A4	833	CLA	CMB-C2B-C3B	2.09	128.69	124.88
14	K6	1401	CLA	CAC-C3C-C4C	2.09	127.71	124.82
14	A2	1607	CLA	C3B-C4B-NB	2.09	111.92	109.21
14	B4	828	CLA	C3B-C4B-NB	2.09	111.92	109.21
16	J5	104	BCR	C33-C5-C6	2.09	126.85	124.51
17	A3	854	LHG	O2-C2-C3	2.09	117.04	109.42
14	B3	1822	CLA	CMB-C2B-C3B	2.09	128.69	124.88
14	A3	835	CLA	CMB-C2B-C3B	2.09	128.69	124.88
14	A1	816	CLA	CMC-C2C-C1C	2.09	128.26	125.05
14	L4	201	CLA	CED-O2D-CGD	2.09	120.80	115.97
16	A2	1651	BCR	C34-C9-C8	2.09	121.44	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F4	203	BCR	C40-C30-C25	2.09	113.70	110.31
14	A2	1633	CLA	CED-O2D-CGD	2.09	120.80	115.97
14	A4	816	CLA	CMB-C2B-C3B	2.10	128.69	124.88
14	B5	1808	CLA	CAC-C3C-C4C	2.10	127.71	124.82
14	A3	810	CLA	CMB-C2B-C3B	2.10	128.70	124.88
14	K1	1401	CLA	CMC-C2C-C1C	2.10	128.26	125.05
14	B2	803	CLA	CMC-C2C-C1C	2.10	128.26	125.05
14	A5	810	CLA	CMC-C2C-C1C	2.10	128.26	125.05
16	B5	1849	BCR	C37-C22-C23	2.10	121.44	118.10
14	B3	1828	CLA	CAC-C3C-C4C	2.10	127.71	124.82
16	B6	845	BCR	C34-C9-C8	2.10	121.44	118.10
14	B3	1801	CLA	CED-O2D-CGD	2.10	120.80	115.97
14	A6	1612	CLA	C3C-C4C-NC	2.10	113.03	110.43
14	A1	809	CLA	CMB-C2B-C3B	2.10	128.70	124.88
14	B5	1840	CLA	CHB-C4A-NA	2.10	127.41	124.51
14	A6	1640	CLA	CAC-C3C-C4C	2.10	127.71	124.82
14	L1	206	CLA	CAC-C3C-C4C	2.10	127.71	124.82
14	A6	1614	CLA	CAC-C3C-C4C	2.10	127.71	124.82
16	A6	1646	BCR	C33-C5-C6	2.10	126.86	124.51
14	B6	834	CLA	C3C-C4C-NC	2.10	113.03	110.43
14	A2	1622	CLA	C3C-C4C-NC	2.10	113.03	110.43
16	B6	846	BCR	C36-C18-C19	2.10	121.44	118.10
19	B1	850	LMG	O7-C10-C11	2.10	115.97	111.55
16	F6	201	BCR	C37-C22-C23	2.10	121.44	118.10
14	A4	811	CLA	C3C-C4C-NC	2.10	113.03	110.43
14	A2	1638	CLA	C1-O2A-CGA	2.10	121.61	116.77
14	J6	1103	CLA	CMC-C2C-C1C	2.10	128.27	125.05
14	K4	1401	CLA	CMC-C2C-C1C	2.10	128.27	125.05
14	B5	1811	CLA	CMC-C2C-C1C	2.10	128.27	125.05
14	A5	840	CLA	C3B-C4B-NB	2.10	111.92	109.21
14	B4	819	CLA	CHB-C4A-NA	2.10	127.42	124.51
14	A5	835	CLA	CMB-C2B-C3B	2.10	128.70	124.88
14	A4	806	CLA	CMC-C2C-C1C	2.10	128.27	125.05
16	F6	201	BCR	C32-C1-C6	2.10	113.71	110.31
14	B1	809	CLA	C3C-C4C-NC	2.10	113.03	110.43
14	A2	1627	CLA	CED-O2D-CGD	2.10	120.81	115.97
14	B4	806	CLA	C3B-C4B-NB	2.10	111.93	109.21
14	B4	840	CLA	C3C-C4C-NC	2.10	113.03	110.43
14	A3	830	CLA	CMC-C2C-C1C	2.10	128.27	125.05
14	A4	810	CLA	CMC-C2C-C1C	2.10	128.27	125.05
14	A5	817	CLA	CMC-C2C-C1C	2.10	128.27	125.05
14	A4	822	CLA	CAC-C3C-C4C	2.10	127.72	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F6	203	BCR	C36-C18-C19	2.10	121.45	118.10
16	A4	846	BCR	C36-C18-C19	2.10	121.45	118.10
14	B1	827	CLA	C4A-NA-C1A	2.10	109.03	106.32
14	A5	817	CLA	CMB-C2B-C3B	2.10	128.71	124.88
19	B2	848	LMG	O7-C10-C11	2.10	115.98	111.55
14	A5	801	CLA	CHB-C4A-NA	2.10	127.42	124.51
14	A6	1611	CLA	CMC-C2C-C1C	2.10	128.27	125.05
14	B1	840	CLA	CMC-C2C-C1C	2.10	128.27	125.05
14	B4	819	CLA	CAC-C3C-C4C	2.10	127.72	124.82
14	B2	806	CLA	C3C-C4C-NC	2.10	113.03	110.43
16	B3	1846	BCR	C1-C6-C7	2.10	121.64	115.73
16	L2	208	BCR	C29-C30-C25	2.10	113.77	110.48
14	A5	834	CLA	CMB-C2B-C3B	2.10	128.71	124.88
14	A4	811	CLA	C4A-NA-C1A	2.10	109.04	106.32
14	B1	838	CLA	C1-O2A-CGA	2.10	121.62	116.77
14	B1	811	CLA	CMC-C2C-C1C	2.10	128.27	125.05
14	B5	1835	CLA	CED-O2D-CGD	2.10	120.82	115.97
14	B6	828	CLA	CED-O2D-CGD	2.11	120.82	115.97
14	B4	805	CLA	CAC-C3C-C4C	2.11	127.72	124.82
14	A6	1631	CLA	CMC-C2C-C1C	2.11	128.28	125.05
14	A1	816	CLA	CMB-C2B-C3B	2.11	128.71	124.88
14	A1	828	CLA	C3B-C4B-NB	2.11	111.93	109.21
14	B3	1809	CLA	C3C-C4C-NC	2.11	113.04	110.43
14	A4	830	CLA	C3C-C4C-NC	2.11	113.04	110.43
14	B1	822	CLA	CED-O2D-CGD	2.11	120.82	115.97
14	B2	814	CLA	CMB-C2B-C3B	2.11	128.72	124.88
16	A5	846	BCR	C33-C5-C6	2.11	126.87	124.51
14	X4	102	CLA	CMB-C2B-C3B	2.11	128.72	124.88
14	B4	822	CLA	C3C-C4C-NC	2.11	113.04	110.43
16	F3	203	BCR	C36-C18-C19	2.11	121.46	118.10
14	A6	1601	CLA	CMC-C2C-C1C	2.11	128.28	125.05
14	A5	840	CLA	CMC-C2C-C1C	2.11	128.28	125.05
14	B3	1830	CLA	CED-O2D-CGD	2.11	120.83	115.97
16	I3	101	BCR	C34-C9-C8	2.11	121.46	118.10
14	B2	807	CLA	CHB-C4A-NA	2.11	127.43	124.51
14	A2	1632	CLA	CMC-C2C-C1C	2.11	128.28	125.05
14	B1	813	CLA	CMC-C2C-C1C	2.11	128.28	125.05
14	J2	101	CLA	CMC-C2C-C1C	2.11	128.28	125.05
14	B5	1842	CLA	C3B-C4B-NB	2.11	111.94	109.21
14	B1	810	CLA	C3B-C4B-NB	2.11	111.94	109.21
14	X5	101	CLA	C4A-NA-C1A	2.11	109.04	106.32
14	A5	838	CLA	CMC-C2C-C1C	2.11	128.28	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	827	CLA	C2C-C1C-NC	2.11	112.27	110.09
14	B3	1823	CLA	CED-O2D-CGD	2.11	120.83	115.97
14	B2	818	CLA	CAC-C3C-C4C	2.11	127.73	124.82
14	B4	838	CLA	C4A-NA-C1A	2.11	109.04	106.32
14	A6	1602	CLA	CGD-CBD-CAD	2.11	117.57	110.73
14	L2	206	CLA	CAC-C3C-C4C	2.11	127.73	124.82
14	A1	810	CLA	CMC-C2C-C1C	2.11	128.28	125.05
16	A2	1650	BCR	C38-C26-C25	2.11	126.87	124.51
14	B1	834	CLA	CED-O2D-CGD	2.11	120.83	115.97
16	A3	850	BCR	C36-C18-C19	2.11	121.46	118.10
14	A5	841	CLA	CMB-C2B-C3B	2.11	128.72	124.88
14	A4	822	CLA	CMB-C2B-C3B	2.11	128.72	124.88
14	B1	837	CLA	CED-O2D-CGD	2.11	120.84	115.97
14	B3	1841	CLA	CMC-C2C-C1C	2.11	128.29	125.05
16	B1	847	BCR	C37-C22-C23	2.11	121.46	118.10
14	B3	1827	CLA	C3B-C4B-NB	2.11	111.94	109.21
14	B5	1812	CLA	CAC-C3C-C4C	2.11	127.73	124.82
14	J6	1102	CLA	CED-O2D-CGD	2.11	120.84	115.97
14	A2	1625	CLA	CMB-C2B-C3B	2.11	128.73	124.88
14	A4	839	CLA	CMC-C2C-C1C	2.11	128.29	125.05
14	B1	827	CLA	CAC-C3C-C4C	2.11	127.73	124.82
14	A3	838	CLA	CAC-C3C-C4C	2.11	127.73	124.82
14	A1	830	CLA	C3C-C4C-NC	2.11	113.05	110.43
16	B6	847	BCR	C34-C9-C8	2.11	121.47	118.10
14	A5	835	CLA	C4A-NA-C1A	2.11	109.05	106.32
14	A5	815	CLA	CED-O2D-CGD	2.11	120.84	115.97
14	A3	835	CLA	CED-O2D-CGD	2.11	120.84	115.97
14	B6	831	CLA	CED-O2D-CGD	2.11	120.84	115.97
14	L5	203	CLA	CED-O2D-CGD	2.12	120.84	115.97
14	A4	808	CLA	CMC-C2C-C1C	2.12	128.29	125.05
14	B3	1810	CLA	C3B-C4B-NB	2.12	111.94	109.21
14	B5	1818	CLA	CMB-C2B-C3B	2.12	128.73	124.88
14	B1	834	CLA	C4A-NA-C1A	2.12	109.05	106.32
16	A5	847	BCR	C40-C30-C25	2.12	113.74	110.31
14	B4	852	CLA	CMB-C2B-C3B	2.12	128.73	124.88
14	B2	811	CLA	C3C-C4C-NC	2.12	113.05	110.43
14	A6	1623	CLA	CAC-C3C-C4C	2.12	127.74	124.82
14	J1	101	CLA	CMB-C2B-C3B	2.12	128.73	124.88
14	L4	201	CLA	CMC-C2C-C1C	2.12	128.29	125.05
14	B5	1828	CLA	C3B-C4B-NB	2.12	111.95	109.21
14	A3	812	CLA	C3C-C4C-NC	2.12	113.05	110.43
14	J3	101	CLA	CED-O2D-CGD	2.12	120.85	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	X2	1701	CLA	CMC-C2C-C1C	2.12	128.29	125.05
14	B3	1825	CLA	CAC-C3C-C4C	2.12	127.74	124.82
14	L4	204	CLA	CAC-C3C-C4C	2.12	127.74	124.82
14	B3	1824	CLA	CAC-C3C-C4C	2.12	127.74	124.82
14	B6	822	CLA	CAC-C3C-C4C	2.12	127.74	124.82
14	A4	818	CLA	CAC-C3C-C4C	2.12	127.74	124.82
14	L3	202	CLA	CMC-C2C-C1C	2.12	128.30	125.05
14	K2	1401	CLA	CMC-C2C-C1C	2.12	128.30	125.05
14	A3	829	CLA	C3B-C4B-NB	2.12	111.95	109.21
14	A1	838	CLA	CED-O2D-CGD	2.12	120.85	115.97
14	A1	821	CLA	CMB-C2B-C3B	2.12	128.74	124.88
14	M2	1201	CLA	C3B-C4B-NB	2.12	111.95	109.21
14	A1	839	CLA	CHB-C4A-NA	2.12	127.44	124.51
16	B2	843	BCR	C37-C22-C23	2.12	121.48	118.10
14	A5	816	CLA	CMB-C2B-C3B	2.12	128.74	124.88
16	B5	1848	BCR	C38-C26-C25	2.12	126.88	124.51
14	A3	813	CLA	C4A-NA-C1A	2.12	109.06	106.32
14	A1	806	CLA	CAC-C3C-C4C	2.12	127.75	124.82
16	B3	1846	BCR	C33-C5-C6	2.12	126.88	124.51
16	B5	1848	BCR	C36-C18-C19	2.12	121.48	118.10
14	B1	806	CLA	CHB-C4A-NA	2.12	127.45	124.51
14	A2	1633	CLA	C3C-C4C-NC	2.12	113.06	110.43
14	B2	820	CLA	CED-O2D-CGD	2.12	120.86	115.97
14	J4	101	CLA	CMC-C2C-C1C	2.12	128.30	125.05
14	B4	802	CLA	O2D-CGD-CBD	2.12	115.05	111.28
14	A5	840	CLA	C4-C3-C5	2.12	118.48	115.96
14	A6	1610	CLA	CMC-C2C-C1C	2.12	128.30	125.05
14	L4	204	CLA	C3B-C4B-NB	2.12	111.96	109.21
14	B4	833	CLA	CED-O2D-CGD	2.12	120.86	115.97
14	B5	1820	CLA	C3C-C4C-NC	2.12	113.06	110.43
14	A5	838	CLA	CED-O2D-CGD	2.12	120.86	115.97
14	A3	822	CLA	CED-O2D-CGD	2.12	120.87	115.97
14	A1	833	CLA	CMB-C2B-C3B	2.12	128.75	124.88
14	A4	830	CLA	C2C-C1C-NC	2.13	112.29	110.09
16	L2	203	BCR	C32-C1-C6	2.13	113.75	110.31
14	B1	808	CLA	C3C-C4C-NC	2.13	113.06	110.43
14	B5	1805	CLA	CMB-C2B-C3B	2.13	128.75	124.88
14	B2	830	CLA	CMB-C2B-C3B	2.13	128.75	124.88
14	B5	1817	CLA	CMB-C2B-C3B	2.13	128.75	124.88
14	A6	1640	CLA	C6-C5-C3	2.13	117.97	112.82
14	B6	820	CLA	C3C-C4C-NC	2.13	113.06	110.43
14	B4	841	CLA	CED-O2D-CGD	2.13	120.87	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	841	CLA	CMB-C2B-C3B	2.13	128.75	124.88
14	A5	807	CLA	CAC-C3C-C4C	2.13	127.75	124.82
14	B5	1830	CLA	CED-O2D-CGD	2.13	120.87	115.97
14	B3	1812	CLA	CMC-C2C-C1C	2.13	128.31	125.05
16	A2	1650	BCR	C33-C5-C6	2.13	126.89	124.51
14	B4	810	CLA	CHB-C4A-NA	2.13	127.45	124.51
14	F1	1301	CLA	CED-O2D-CGD	2.13	120.87	115.97
14	B5	1841	CLA	CMC-C2C-C1C	2.13	128.31	125.05
14	A3	841	CLA	CMC-C2C-C1C	2.13	128.31	125.05
14	B4	816	CLA	CED-O2D-CGD	2.13	120.88	115.97
14	A1	805	CLA	CAC-C3C-C4C	2.13	127.76	124.82
14	B4	825	CLA	CAC-C3C-C4C	2.13	127.76	124.82
14	J3	101	CLA	CMC-C2C-C1C	2.13	128.31	125.05
14	A5	823	CLA	CMB-C2B-C3B	2.13	128.76	124.88
14	B4	852	CLA	C2C-C1C-NC	2.13	112.30	110.09
14	A3	811	CLA	C3B-C4B-NB	2.13	111.96	109.21
14	B3	1816	CLA	CMC-C2C-C1C	2.13	128.31	125.05
14	A3	838	CLA	C11-C10-C8	2.13	122.73	115.73
14	A1	818	CLA	CAC-C3C-C4C	2.13	127.76	124.82
14	B5	1808	CLA	C11-C10-C8	2.13	122.73	115.73
14	A1	826	CLA	C4A-NA-C1A	2.13	109.07	106.32
14	B5	1818	CLA	CED-O2D-CGD	2.13	120.88	115.97
14	B4	811	CLA	CED-O2D-CGD	2.13	120.88	115.97
14	B2	815	CLA	CED-O2D-CGD	2.13	120.88	115.97
14	X1	1701	CLA	C4A-NA-C1A	2.13	109.07	106.32
14	B5	1801	CLA	CMC-C2C-C1C	2.13	128.32	125.05
14	B4	802	CLA	C3C-C4C-NC	2.13	113.07	110.43
14	M1	1201	CLA	C3B-C4B-NB	2.13	111.97	109.21
14	A4	840	CLA	C6-C5-C3	2.13	117.99	112.82
14	A1	818	CLA	C3C-C4C-NC	2.13	113.07	110.43
14	B6	808	CLA	CHB-C4A-NA	2.13	127.46	124.51
14	A2	1608	CLA	CAC-C3C-C4C	2.13	127.76	124.82
14	A5	811	CLA	C3B-C4B-NB	2.13	111.97	109.21
14	B2	811	CLA	CMC-C2C-C1C	2.13	128.32	125.05
14	A6	1629	CLA	CAC-C3C-C4C	2.13	127.76	124.82
14	B6	805	CLA	CHB-C4A-NA	2.13	127.46	124.51
14	B4	819	CLA	CMB-C2B-C3B	2.13	128.77	124.88
14	A4	818	CLA	C3C-C4C-NC	2.13	113.07	110.43
14	A1	821	CLA	CED-O2D-CGD	2.14	120.89	115.97
14	B1	811	CLA	C3B-C4B-NB	2.14	111.97	109.21
14	A4	841	CLA	CED-O2D-CGD	2.14	120.89	115.97
14	B1	854	CLA	CAC-C3C-C4C	2.14	127.77	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A3	850	BCR	C33-C5-C6	2.14	126.90	124.51
16	A2	1648	BCR	C33-C5-C6	2.14	126.90	124.51
14	A5	803	CLA	C3C-C4C-NC	2.14	113.07	110.43
14	L2	206	CLA	C3C-C4C-NC	2.14	113.08	110.43
14	A2	1608	CLA	C3C-C4C-NC	2.14	113.08	110.43
16	B5	1849	BCR	C29-C30-C25	2.14	113.82	110.48
14	B4	831	CLA	C9-C8-C10	2.14	119.14	111.36
14	B1	832	CLA	CMB-C2B-C3B	2.14	128.77	124.88
14	A2	1635	CLA	CMB-C2B-C3B	2.14	128.77	124.88
14	A5	836	CLA	CMC-C2C-C1C	2.14	128.33	125.05
14	A3	804	CLA	CMC-C2C-C1C	2.14	128.33	125.05
14	A2	1636	CLA	CMB-C2B-C3B	2.14	128.77	124.88
14	B6	827	CLA	CMB-C2B-C3B	2.14	128.78	124.88
14	B6	814	CLA	CED-O2D-CGD	2.14	120.90	115.97
14	A2	1640	CLA	CAC-C3C-C4C	2.14	127.77	124.82
14	A5	831	CLA	CMC-C2C-C1C	2.14	128.33	125.05
14	B4	824	CLA	C3C-C4C-NC	2.14	113.08	110.43
14	B4	814	CLA	C3C-C4C-NC	2.14	113.08	110.43
14	B3	1812	CLA	C4A-NA-C1A	2.14	109.08	106.32
16	B4	849	BCR	C30-C25-C24	2.14	121.74	115.73
14	B3	1820	CLA	CED-O2D-CGD	2.14	120.90	115.97
14	A3	814	CLA	CAC-C3C-C4C	2.14	127.77	124.82
14	A5	802	CLA	CMB-C2B-C3B	2.14	128.78	124.88
14	B4	818	CLA	CMB-C2B-C3B	2.14	128.78	124.88
14	B5	1829	CLA	CMB-C2B-C3B	2.14	128.78	124.88
14	L6	207	CLA	C3B-C4B-NB	2.14	111.98	109.21
14	J3	101	CLA	C4A-NA-C1A	2.14	109.08	106.32
14	B3	1817	CLA	CMC-C2C-C1C	2.14	128.33	125.05
14	A1	817	CLA	CAC-C3C-C4C	2.14	127.77	124.82
16	B2	844	BCR	C28-C27-C26	2.14	117.75	113.99
14	B3	1811	CLA	C3B-C4B-NB	2.14	111.98	109.21
14	B5	1801	CLA	C1-C2-C3	2.14	129.90	125.96
14	B2	808	CLA	CMC-C2C-C1C	2.14	128.33	125.05
14	B5	1809	CLA	C3C-C4C-NC	2.14	113.08	110.43
14	B3	1829	CLA	CMB-C2B-C3B	2.14	128.78	124.88
14	B4	815	CLA	CED-O2D-CGD	2.14	120.91	115.97
14	B5	1816	CLA	CED-O2D-CGD	2.14	120.91	115.97
14	A2	1638	CLA	C4A-NA-C1A	2.14	109.09	106.32
14	F3	202	CLA	CAC-C3C-C4C	2.14	127.78	124.82
14	A5	837	CLA	CAC-C3C-C4C	2.14	127.78	124.82
14	B2	801	CLA	CMC-C2C-C1C	2.14	128.34	125.05
16	I4	101	BCR	C34-C9-C8	2.14	121.52	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A1	813	CLA	CAC-C3C-C4C	2.14	127.78	124.82
14	B2	835	CLA	CAC-C3C-C4C	2.15	127.78	124.82
14	A4	839	CLA	CAC-C3C-C4C	2.15	127.78	124.82
14	A6	1637	CLA	CED-O2D-CGD	2.15	120.91	115.97
14	J5	102	CLA	C3C-C4C-NC	2.15	113.09	110.43
14	A4	853	CLA	CMC-C2C-C1C	2.15	128.34	125.05
14	A2	1614	CLA	C3C-C4C-NC	2.15	113.09	110.43
14	A3	838	CLA	C9-C8-C7	2.15	119.17	111.36
14	A5	841	CLA	CED-O2D-CGD	2.15	120.92	115.97
14	B5	1828	CLA	CAC-C3C-C4C	2.15	127.78	124.82
14	B3	1827	CLA	CHB-C4A-NA	2.15	127.48	124.51
14	A2	1617	CLA	CED-O2D-CGD	2.15	120.92	115.97
14	L2	207	CLA	CAC-C3C-C4C	2.15	127.78	124.82
16	L2	203	BCR	C38-C26-C25	2.15	126.91	124.51
14	A2	1644	CLA	CHB-C4A-NA	2.15	127.48	124.51
16	B1	845	BCR	C40-C30-C25	2.15	113.79	110.31
14	A1	834	CLA	CAC-C3C-C4C	2.15	127.78	124.82
14	A3	821	CLA	CAC-C3C-C4C	2.15	127.78	124.82
14	A4	828	CLA	C3B-C4B-NB	2.15	111.99	109.21
14	B2	832	CLA	CED-O2D-CGD	2.15	120.92	115.97
14	B5	1830	CLA	C5-C3-C2	2.15	125.47	121.10
14	A2	1611	CLA	CMC-C2C-C1C	2.15	128.34	125.05
14	B1	824	CLA	CMC-C2C-C1C	2.15	128.34	125.05
14	B3	1841	CLA	CMB-C2B-C3B	2.15	128.80	124.88
14	B6	836	CLA	CED-O2D-CGD	2.15	120.93	115.97
14	A5	822	CLA	CED-O2D-CGD	2.15	120.93	115.97
16	B5	1846	BCR	C37-C22-C23	2.15	121.53	118.10
16	I6	102	BCR	C37-C22-C23	2.15	121.53	118.10
14	A1	822	CLA	CMB-C2B-C3B	2.15	128.80	124.88
14	A3	802	CLA	CED-O2D-CGD	2.15	120.93	115.97
14	A6	1629	CLA	C3B-C4B-NB	2.15	111.99	109.21
14	A4	815	CLA	CMB-C2B-C3B	2.15	128.80	124.88
14	J2	101	CLA	CED-O2D-CGD	2.15	120.93	115.97
14	A6	1631	CLA	C3C-C4C-NC	2.15	113.10	110.43
14	A1	802	CLA	CMC-C2C-C1C	2.15	128.35	125.05
14	A3	845	CLA	CMB-C2B-C3B	2.15	128.80	124.88
14	B4	804	CLA	CMB-C2B-C3B	2.15	128.80	124.88
14	A2	1623	CLA	CAC-C3C-C4C	2.15	127.79	124.82
14	B5	1840	CLA	C3C-C4C-NC	2.16	113.10	110.43
14	A6	1605	CLA	C3B-C4B-NB	2.16	112.00	109.21
17	A1	849	LHG	O2-C2-C3	2.16	117.26	109.42
14	A6	1620	CLA	C2C-C1C-NC	2.16	112.32	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1633	CLA	CED-O2D-CGD	2.16	120.94	115.97
14	B3	1805	CLA	CAC-C3C-C4C	2.16	127.79	124.82
14	A3	839	CLA	CAC-C3C-C4C	2.16	127.79	124.82
14	B2	822	CLA	CAC-C3C-C4C	2.16	127.79	124.82
14	A1	815	CLA	CMB-C2B-C3B	2.16	128.81	124.88
14	B2	816	CLA	CMB-C2B-C3B	2.16	128.81	124.88
14	B1	804	CLA	CMC-C2C-C1C	2.16	128.35	125.05
14	A3	843	CLA	CHB-C4A-NA	2.16	127.49	124.51
16	B2	844	BCR	C38-C26-C25	2.16	126.92	124.51
14	A1	840	CLA	C3C-C4C-NC	2.16	113.10	110.43
14	B4	828	CLA	CAC-C3C-C4C	2.16	127.80	124.82
14	B5	1811	CLA	C3B-C4B-NB	2.16	112.00	109.21
14	A6	1635	CLA	CMB-C2B-C3B	2.16	128.81	124.88
16	B5	1846	BCR	C36-C18-C19	2.16	121.54	118.10
14	A6	1609	CLA	CAA-C2A-C1A	2.16	119.05	111.97
14	A4	824	CLA	CED-O2D-CGD	2.16	120.95	115.97
14	A1	823	CLA	CAC-C3C-C4C	2.16	127.80	124.82
14	A3	841	CLA	C4-C3-C5	2.16	118.52	115.96
14	A5	809	CLA	CMC-C2C-C1C	2.16	128.36	125.05
14	B1	828	CLA	CED-O2D-CGD	2.16	120.95	115.97
14	F1	1301	CLA	CAC-C3C-C4C	2.16	127.80	124.82
14	A1	811	CLA	C4A-NA-C1A	2.16	109.11	106.32
14	A4	805	CLA	C11-C10-C8	2.16	122.83	115.73
14	A1	838	CLA	CMB-C2B-C3B	2.16	128.81	124.88
16	B6	845	BCR	C28-C27-C26	2.16	117.78	113.99
14	A4	826	CLA	CMC-C2C-C1C	2.16	128.36	125.05
14	A2	1613	CLA	CMC-C2C-C1C	2.16	128.36	125.05
14	A2	1618	CLA	CMB-C2B-C3B	2.16	128.82	124.88
16	M1	1202	BCR	C33-C5-C6	2.16	126.93	124.51
14	B2	834	CLA	CMC-C2C-C1C	2.16	128.36	125.05
14	A3	807	CLA	CMC-C2C-C1C	2.16	128.36	125.05
16	B5	1847	BCR	C28-C27-C26	2.16	117.79	113.99
14	A6	1639	CLA	C4-C3-C5	2.16	118.52	115.96
14	B3	1818	CLA	CED-O2D-CGD	2.16	120.95	115.97
14	A1	822	CLA	CAC-C3C-C4C	2.16	127.80	124.82
14	B6	810	CLA	CMC-C2C-C1C	2.16	128.37	125.05
14	B3	1826	CLA	CMC-C2C-C1C	2.16	128.37	125.05
14	A5	843	CLA	CMC-C2C-C1C	2.16	128.37	125.05
14	A4	832	CLA	CMB-C2B-C3B	2.16	128.82	124.88
14	A6	1603	CLA	C3C-C4C-NC	2.16	113.11	110.43
14	B6	805	CLA	C3C-C4C-NC	2.16	113.11	110.43
14	A5	811	CLA	CMC-C2C-C1C	2.16	128.37	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1827	CLA	CHB-C4A-NA	2.16	127.50	124.51
16	A5	846	BCR	C38-C26-C25	2.16	126.93	124.51
14	B5	1814	CLA	CAC-C3C-C4C	2.16	127.81	124.82
14	B5	1833	CLA	CMB-C2B-C3B	2.16	128.82	124.88
14	B5	1823	CLA	C3C-C4C-NC	2.17	113.11	110.43
14	B1	802	CLA	C3C-C4C-NC	2.17	113.11	110.43
16	B2	850	BCR	C37-C22-C23	2.17	121.55	118.10
14	A5	809	CLA	C4A-NA-C1A	2.17	109.12	106.32
14	A2	1614	CLA	C4A-NA-C1A	2.17	109.12	106.32
14	B6	821	CLA	C3C-C4C-NC	2.17	113.11	110.43
14	B1	826	CLA	CHB-C4A-NA	2.17	127.51	124.51
16	B5	1847	BCR	C34-C9-C8	2.17	121.55	118.10
14	L1	206	CLA	C3C-C4C-NC	2.17	113.11	110.43
14	B6	812	CLA	C3C-C4C-NC	2.17	113.11	110.43
14	B6	825	CLA	CHB-C4A-NA	2.17	127.51	124.51
14	L5	202	CLA	CMC-C2C-C1C	2.17	128.37	125.05
16	B1	846	BCR	C38-C26-C25	2.17	126.94	124.51
17	A4	851	LHG	C25-C24-C23	2.17	124.94	114.17
14	B2	809	CLA	CAC-C3C-C4C	2.17	127.81	124.82
14	A2	1605	CLA	C3C-C4C-NC	2.17	113.12	110.43
14	B1	821	CLA	CED-O2D-CGD	2.17	120.97	115.97
14	A4	810	CLA	C3B-C4B-NB	2.17	112.02	109.21
16	F6	201	BCR	C35-C13-C12	2.17	121.56	118.10
14	A2	1613	CLA	C3B-C4B-NB	2.17	112.02	109.21
14	M3	1601	CLA	CMC-C2C-C1C	2.17	128.38	125.05
14	A2	1637	CLA	CMB-C2B-C3B	2.17	128.83	124.88
14	A3	834	CLA	CMC-C2C-C1C	2.17	128.38	125.05
14	B3	1818	CLA	CMB-C2B-C3B	2.17	128.84	124.88
14	A6	1623	CLA	CMB-C2B-C3B	2.17	128.84	124.88
14	B4	817	CLA	CMB-C2B-C3B	2.17	128.84	124.88
14	B2	801	CLA	CED-O2D-CGD	2.17	120.97	115.97
16	B5	1847	BCR	C40-C30-C25	2.17	113.83	110.31
14	A3	833	CLA	CMB-C2B-C3B	2.17	128.84	124.88
14	A1	834	CLA	CMC-C2C-C1C	2.17	128.38	125.05
14	B3	1803	CLA	CMC-C2C-C1C	2.17	128.38	125.05
14	A1	814	CLA	C3C-C4C-NC	2.17	113.12	110.43
16	J5	103	BCR	C35-C13-C12	2.17	121.56	118.10
14	A6	1640	CLA	CMB-C2B-C3B	2.17	128.84	124.88
14	A2	1644	CLA	CED-O2D-CGD	2.17	120.98	115.97
14	B2	828	CLA	CAC-C3C-C4C	2.17	127.82	124.82
14	L4	204	CLA	C3C-C4C-NC	2.17	113.12	110.43
14	A2	1629	CLA	CMC-C2C-C1C	2.18	128.38	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1636	CLA	C4A-NA-C1A	2.18	109.13	106.32
14	B6	816	CLA	CMB-C2B-C3B	2.18	128.84	124.88
16	B3	1846	BCR	C36-C18-C19	2.18	121.56	118.10
14	A2	1644	CLA	CAC-C3C-C4C	2.18	127.82	124.82
14	B2	801	CLA	CHB-C4A-NA	2.18	127.52	124.51
14	B2	820	CLA	C3C-C4C-NC	2.18	113.12	110.43
14	A2	1621	CLA	C3C-C4C-NC	2.18	113.12	110.43
14	A5	818	CLA	CED-O2D-CGD	2.18	120.98	115.97
14	B1	818	CLA	CHB-C4A-NA	2.18	127.52	124.51
14	A3	821	CLA	C11-C10-C8	2.18	122.88	115.73
14	B5	1814	CLA	C3C-C4C-NC	2.18	113.12	110.43
14	B4	822	CLA	CED-O2D-CGD	2.18	120.99	115.97
17	A2	1654	LHG	O2-C2-C3	2.18	117.34	109.42
14	A3	803	CLA	CMC-C2C-C1C	2.18	128.39	125.05
14	A4	840	CLA	CMB-C2B-C3B	2.18	128.85	124.88
14	A3	845	CLA	C1-C2-C3	2.18	129.97	125.96
14	B3	1812	CLA	CAA-C2A-C1A	2.18	119.12	111.97
14	B3	1831	CLA	CMC-C2C-C1C	2.18	128.39	125.05
14	B2	825	CLA	CAC-C3C-C4C	2.18	127.83	124.82
14	B1	839	CLA	C3C-C4C-NC	2.18	113.13	110.43
14	A4	830	CLA	CED-O2D-CGD	2.18	120.99	115.97
14	B5	1827	CLA	C3B-C4B-NB	2.18	112.03	109.21
14	A6	1621	CLA	CAC-C3C-C4C	2.18	127.83	124.82
14	B4	826	CLA	C4-C3-C5	2.18	119.05	115.29
14	A3	842	CLA	CMB-C2B-C3B	2.18	128.85	124.88
14	B4	806	CLA	CMC-C2C-C1C	2.18	128.40	125.05
14	B6	816	CLA	CED-O2D-CGD	2.18	121.00	115.97
14	A2	1633	CLA	C2C-C1C-NC	2.18	112.35	110.09
14	A3	809	CLA	CMB-C2B-C3B	2.18	128.86	124.88
14	B1	817	CLA	CED-O2D-CGD	2.18	121.00	115.97
14	B4	803	CLA	CMC-C2C-C1C	2.18	128.40	125.05
14	B3	1801	CLA	CMB-C2B-C3B	2.18	128.86	124.88
16	B1	846	BCR	C36-C18-C19	2.19	121.58	118.10
14	A1	833	CLA	CMC-C2C-C1C	2.19	128.40	125.05
16	B6	846	BCR	C38-C26-C25	2.19	126.95	124.51
14	B5	1803	CLA	CHB-C4A-NA	2.19	127.53	124.51
14	A1	801	CLA	CGD-CBD-CAD	2.19	117.81	110.73
14	A5	841	CLA	C6-C5-C3	2.19	118.12	112.82
14	B3	1819	CLA	CAC-C3C-C4C	2.19	127.83	124.82
14	A4	802	CLA	C3C-C4C-NC	2.19	113.14	110.43
14	A3	811	CLA	CMC-C2C-C1C	2.19	128.40	125.05
14	A5	812	CLA	C4A-NA-C1A	2.19	109.14	106.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1837	CLA	CED-O2D-CGD	2.19	121.01	115.97
14	B2	819	CLA	C3C-C4C-NC	2.19	113.14	110.43
14	A5	815	CLA	C3B-C4B-NB	2.19	112.04	109.21
14	X1	1701	CLA	CMC-C2C-C1C	2.19	128.40	125.05
14	A1	837	CLA	C4-C3-C5	2.19	118.56	115.96
14	A6	1632	CLA	CMB-C2B-C3B	2.19	128.87	124.88
14	A3	803	CLA	C3C-C4C-NC	2.19	113.14	110.43
14	A3	842	CLA	C6-C5-C3	2.19	118.13	112.82
14	A1	824	CLA	CMC-C2C-C1C	2.19	128.41	125.05
14	A6	1619	CLA	CED-O2D-CGD	2.19	121.02	115.97
14	B6	813	CLA	C3B-C4B-NB	2.19	112.04	109.21
14	B2	824	CLA	C3C-C4C-NC	2.19	113.14	110.43
14	A1	806	CLA	CMC-C2C-C1C	2.19	128.41	125.05
16	I1	103	BCR	C29-C30-C25	2.19	113.90	110.48
14	B6	802	CLA	CMC-C2C-C1C	2.19	128.41	125.05
14	A4	805	CLA	CAC-C3C-C4C	2.19	127.84	124.82
16	A1	844	BCR	C40-C30-C25	2.19	113.86	110.31
16	B6	847	BCR	C37-C22-C23	2.19	121.59	118.10
14	A5	803	CLA	CMC-C2C-C1C	2.19	128.41	125.05
14	F4	202	CLA	CAC-C3C-C4C	2.19	127.84	124.82
14	A2	1622	CLA	C2C-C1C-NC	2.19	112.36	110.09
14	A4	813	CLA	CAC-C3C-C4C	2.19	127.84	124.82
14	B1	853	CLA	CMB-C2B-C3B	2.19	128.87	124.88
14	B2	830	CLA	CED-O2D-CGD	2.19	121.03	115.97
17	A2	1654	LHG	C25-C24-C23	2.19	125.07	114.17
14	K4	1401	CLA	CAC-C3C-C4C	2.19	127.85	124.82
14	B2	835	CLA	CED-O2D-CGD	2.19	121.03	115.97
14	A4	803	CLA	CMC-C2C-C1C	2.19	128.41	125.05
14	B3	1806	CLA	CMC-C2C-C1C	2.19	128.41	125.05
14	B6	823	CLA	CAC-C3C-C4C	2.20	127.85	124.82
14	A2	1634	CLA	CED-O2D-CGD	2.20	121.03	115.97
14	B2	812	CLA	C3B-C4B-NB	2.20	112.05	109.21
14	A4	841	CLA	CHB-C4A-NA	2.20	127.55	124.51
14	A1	819	CLA	C1-O2A-CGA	2.20	121.83	116.77
14	J1	102	CLA	C3C-C4C-NC	2.20	113.15	110.43
14	A5	843	CLA	CMB-C2B-C3B	2.20	128.88	124.88
14	B4	827	CLA	CHB-C4A-NA	2.20	127.55	124.51
14	B6	835	CLA	CMB-C2B-C3B	2.20	128.88	124.88
14	A3	845	CLA	CMC-C2C-C1C	2.20	128.42	125.05
14	B3	1830	CLA	C5-C3-C2	2.20	125.57	121.10
14	A6	1618	CLA	CAC-C3C-C4C	2.20	127.85	124.82
14	B4	838	CLA	CED-O2D-CGD	2.20	121.04	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	820	CLA	C3C-C4C-NC	2.20	113.15	110.43
14	A3	844	CLA	C3C-C4C-NC	2.20	113.15	110.43
14	A5	819	CLA	CAC-C3C-C4C	2.20	127.85	124.82
16	B4	846	BCR	C36-C18-C19	2.20	121.60	118.10
14	B3	1817	CLA	CMB-C2B-C3B	2.20	128.89	124.88
14	B2	823	CLA	C4-C3-C5	2.20	119.08	115.29
14	K1	1401	CLA	CAC-C3C-C4C	2.20	127.86	124.82
14	B5	1802	CLA	C3C-C4C-NC	2.20	113.15	110.43
14	B4	827	CLA	C3B-C4B-NB	2.20	112.06	109.21
14	A5	804	CLA	CMC-C2C-C1C	2.20	128.42	125.05
14	A4	834	CLA	CMB-C2B-C3B	2.20	128.89	124.88
14	J6	1101	CLA	C3C-C4C-NC	2.20	113.16	110.43
14	L3	205	CLA	CAC-C3C-C4C	2.20	127.86	124.82
14	B4	812	CLA	CAA-C2A-C1A	2.20	119.19	111.97
16	J2	102	BCR	C35-C13-C12	2.20	121.61	118.10
14	L3	204	CLA	C3B-C4B-NB	2.20	112.06	109.21
14	A3	826	CLA	C9-C8-C10	2.20	119.38	111.36
16	A4	849	BCR	C34-C9-C8	2.20	121.61	118.10
14	B3	1804	CLA	CMB-C2B-C3B	2.20	128.89	124.88
14	A6	1641	CLA	C3C-C4C-NC	2.20	113.16	110.43
14	B4	837	CLA	CED-O2D-CGD	2.20	121.05	115.97
14	B2	824	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	B4	823	CLA	C3C-C4C-NC	2.21	113.16	110.43
14	B5	1835	CLA	C3C-C4C-NC	2.21	113.16	110.43
14	B6	828	CLA	CAC-C3C-C4C	2.21	127.86	124.82
14	L2	202	CLA	CED-O2D-CGD	2.21	121.05	115.97
14	A1	830	CLA	CED-O2D-CGD	2.21	121.05	115.97
14	A5	842	CLA	CHB-C4A-NA	2.21	127.56	124.51
14	A3	813	CLA	CED-O2D-CGD	2.21	121.05	115.97
14	A1	820	CLA	C3C-C4C-NC	2.21	113.16	110.43
14	A6	1616	CLA	CMB-C2B-C3B	2.21	128.90	124.88
14	B5	1805	CLA	CHB-C4A-NA	2.21	127.56	124.51
14	A4	801	CLA	CHB-C4A-NA	2.21	127.56	124.51
16	B2	845	BCR	C36-C18-C19	2.21	121.61	118.10
16	A3	850	BCR	C38-C26-C25	2.21	126.98	124.51
14	A1	838	CLA	C6-C5-C3	2.21	118.17	112.82
14	A3	806	CLA	C3C-C4C-NC	2.21	113.16	110.43
14	A1	835	CLA	CAC-C3C-C4C	2.21	127.86	124.82
14	B1	823	CLA	C3C-C4C-NC	2.21	113.16	110.43
14	J1	101	CLA	C3C-C4C-NC	2.21	113.16	110.43
16	B6	845	BCR	C40-C30-C25	2.21	113.89	110.31
14	A5	819	CLA	C3B-C4B-NB	2.21	112.07	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1617	CLA	CMC-C2C-C1C	2.21	128.44	125.05
14	B1	825	CLA	C4-C3-C5	2.21	119.10	115.29
14	B3	1801	CLA	CMC-C2C-C1C	2.21	128.44	125.05
14	L6	203	CLA	CHB-C4A-NA	2.21	127.57	124.51
14	A4	821	CLA	CED-O2D-CGD	2.21	121.06	115.97
14	A6	1606	CLA	CAC-C3C-C4C	2.21	127.87	124.82
14	B2	815	CLA	CMB-C2B-C3B	2.21	128.91	124.88
14	A1	815	CLA	CED-O2D-CGD	2.21	121.06	115.97
14	B2	816	CLA	C3C-C4C-NC	2.21	113.17	110.43
14	B4	825	CLA	CMC-C2C-C1C	2.21	128.44	125.05
14	A3	831	CLA	CED-O2D-CGD	2.21	121.06	115.97
14	B1	807	CLA	CHB-C4A-NA	2.21	127.57	124.51
14	A6	1626	CLA	C3B-C4B-NB	2.21	112.07	109.21
14	B4	811	CLA	CMC-C2C-C1C	2.21	128.44	125.05
14	B1	853	CLA	C2C-C1C-NC	2.21	112.38	110.09
16	F4	204	BCR	C37-C22-C23	2.21	121.62	118.10
14	A5	838	CLA	CAC-C3C-C4C	2.21	127.87	124.82
14	B3	1837	CLA	CMB-C2B-C3B	2.21	128.91	124.88
14	B4	852	CLA	CMC-C2C-C1C	2.21	128.44	125.05
14	A2	1645	CLA	C3C-C4C-NC	2.21	113.17	110.43
14	B3	1812	CLA	CAC-C3C-C4C	2.21	127.87	124.82
14	A3	823	CLA	CAC-C3C-C4C	2.21	127.87	124.82
14	A3	843	CLA	CED-O2D-CGD	2.21	121.07	115.97
14	B1	834	CLA	C3C-C4C-NC	2.21	113.17	110.43
14	F2	202	CLA	CAC-C3C-C4C	2.21	127.87	124.82
14	B3	1819	CLA	CHB-C4A-NA	2.21	127.57	124.51
14	B1	817	CLA	CMB-C2B-C3B	2.21	128.91	124.88
14	B1	805	CLA	CMB-C2B-C3B	2.22	128.91	124.88
14	B1	816	CLA	CMB-C2B-C3B	2.22	128.91	124.88
14	A3	841	CLA	CAC-C3C-C4C	2.22	127.88	124.82
14	A3	817	CLA	CMC-C2C-C1C	2.22	128.45	125.05
14	A1	818	CLA	CED-O2D-CGD	2.22	121.08	115.97
14	A3	823	CLA	CMB-C2B-C3B	2.22	128.92	124.88
14	A2	1624	CLA	CED-O2D-CGD	2.22	121.08	115.97
17	A5	852	LHG	C25-C24-C23	2.22	125.18	114.17
14	B5	1837	CLA	CMB-C2B-C3B	2.22	128.92	124.88
14	B4	803	CLA	CHB-C4A-NA	2.22	127.58	124.51
16	L5	207	BCR	C29-C30-C25	2.22	113.94	110.48
14	B1	811	CLA	CED-O2D-CGD	2.22	121.08	115.97
16	B2	846	BCR	C37-C22-C23	2.22	121.63	118.10
14	A1	837	CLA	CAC-C3C-C4C	2.22	127.88	124.82
14	A6	1609	CLA	CMB-C2B-C3B	2.22	128.92	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	826	CLA	C2C-C1C-NC	2.22	112.39	110.09
14	B5	1808	CLA	C3B-C4B-NB	2.22	112.08	109.21
14	B3	1819	CLA	CMB-C2B-C3B	2.22	128.92	124.88
14	B1	836	CLA	CMB-C2B-C3B	2.22	128.92	124.88
14	A3	816	CLA	CMB-C2B-C3B	2.22	128.92	124.88
14	B4	809	CLA	CED-O2D-CGD	2.22	121.09	115.97
14	A4	816	CLA	CMC-C2C-C1C	2.22	128.45	125.05
14	J6	1101	CLA	CMC-C2C-C1C	2.22	128.45	125.05
14	B4	830	CLA	C5-C3-C2	2.22	125.61	121.10
16	B4	847	BCR	C40-C30-C25	2.22	113.91	110.31
14	B2	827	CLA	CAC-C3C-C4C	2.22	127.88	124.82
14	B1	806	CLA	CAC-C3C-C4C	2.22	127.88	124.82
14	A4	842	CLA	C3C-C4C-NC	2.22	113.18	110.43
14	A5	805	CLA	C3B-C4B-NB	2.22	112.08	109.21
14	B1	813	CLA	CED-O2D-CGD	2.22	121.09	115.97
14	A5	825	CLA	CMC-C2C-C1C	2.22	128.45	125.05
14	A3	825	CLA	CMC-C2C-C1C	2.22	128.46	125.05
14	A2	1620	CLA	CAC-C3C-C4C	2.22	127.89	124.82
14	F6	202	CLA	CAC-C3C-C4C	2.22	127.89	124.82
16	B3	1851	BCR	C37-C22-C23	2.22	121.64	118.10
16	M6	1202	BCR	C33-C5-C6	2.22	127.00	124.51
14	A2	1616	CLA	CED-O2D-CGD	2.22	121.09	115.97
14	B6	821	CLA	CED-O2D-CGD	2.22	121.09	115.97
14	B5	1819	CLA	CMB-C2B-C3B	2.22	128.93	124.88
16	M5	101	BCR	C33-C5-C6	2.22	127.00	124.51
14	M6	1201	CLA	C3B-C4B-NB	2.22	112.09	109.21
14	A6	1607	CLA	CMC-C2C-C1C	2.22	128.46	125.05
14	B4	852	CLA	C1-C2-C3	2.23	130.06	125.96
14	B6	822	CLA	C3B-C4B-NB	2.23	112.09	109.21
14	B3	1814	CLA	C3C-C4C-NC	2.23	113.18	110.43
14	B2	825	CLA	C4A-NA-C1A	2.23	109.19	106.32
14	B5	1823	CLA	C4A-NA-C1A	2.23	109.19	106.32
14	B5	1833	CLA	CED-O2D-CGD	2.23	121.10	115.97
14	A6	1635	CLA	CMC-C2C-C1C	2.23	128.46	125.05
14	J4	102	CLA	C3C-C4C-NC	2.23	113.19	110.43
14	B3	1826	CLA	C3C-C4C-NC	2.23	113.19	110.43
14	B5	1822	CLA	C3C-C4C-NC	2.23	113.19	110.43
16	F3	201	BCR	C35-C13-C12	2.23	121.65	118.10
16	L5	201	BCR	C37-C22-C23	2.23	121.65	118.10
16	B3	1849	BCR	C29-C30-C25	2.23	113.96	110.48
14	X4	102	CLA	CMC-C2C-C1C	2.23	128.46	125.05
14	A6	1639	CLA	CMC-C2C-C1C	2.23	128.46	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1616	CLA	CED-O2D-CGD	2.23	121.10	115.97
14	A4	817	CLA	CAC-C3C-C4C	2.23	127.89	124.82
14	B3	1824	CLA	C3C-C4C-NC	2.23	113.19	110.43
14	B6	824	CLA	C4-C3-C5	2.23	119.13	115.29
14	B2	803	CLA	C3C-C4C-NC	2.23	113.19	110.43
14	A6	1603	CLA	CHB-C4A-NA	2.23	127.59	124.51
14	A2	1617	CLA	C3B-C4B-NB	2.23	112.09	109.21
14	A5	826	CLA	C3B-C4B-NB	2.23	112.09	109.21
14	B5	1805	CLA	CAC-C3C-C4C	2.23	127.89	124.82
16	L4	206	BCR	C29-C30-C25	2.23	113.97	110.48
14	A2	1604	CLA	O2D-CGD-CBD	2.23	115.24	111.28
14	A5	804	CLA	CAC-C3C-C4C	2.23	127.90	124.82
14	B1	806	CLA	CMB-C2B-C3B	2.23	128.94	124.88
14	A4	819	CLA	C2C-C1C-NC	2.23	112.40	110.09
14	B5	1806	CLA	CMC-C2C-C1C	2.23	128.47	125.05
14	B4	830	CLA	CAC-C3C-C4C	2.23	127.90	124.82
14	B1	808	CLA	CED-O2D-CGD	2.23	121.11	115.97
14	F2	202	CLA	CED-O2D-CGD	2.23	121.11	115.97
14	B2	821	CLA	C3C-C4C-NC	2.23	113.19	110.43
14	A3	809	CLA	CMC-C2C-C1C	2.23	128.47	125.05
16	F2	201	BCR	C35-C13-C12	2.23	121.66	118.10
16	M2	1202	BCR	C33-C5-C6	2.23	127.01	124.51
14	A5	843	CLA	C1-C2-C3	2.23	130.07	125.96
14	B6	810	CLA	CAA-C2A-C1A	2.23	119.29	111.97
14	B4	841	CLA	CMC-C2C-C1C	2.23	128.47	125.05
14	A5	832	CLA	CMC-C2C-C1C	2.23	128.47	125.05
16	B6	844	BCR	C37-C22-C23	2.23	121.66	118.10
14	B6	807	CLA	C3C-C4C-NC	2.23	113.19	110.43
14	A5	818	CLA	CAC-C3C-C4C	2.23	127.90	124.82
16	L4	206	BCR	C38-C26-C25	2.23	127.01	124.51
14	A6	1619	CLA	CAC-C3C-C4C	2.23	127.90	124.82
14	A2	1616	CLA	C3C-C4C-NC	2.24	113.20	110.43
14	A4	815	CLA	CED-O2D-CGD	2.24	121.12	115.97
16	B2	843	BCR	C33-C5-C6	2.24	127.01	124.51
14	B6	822	CLA	C1-O2A-CGA	2.24	121.92	116.77
14	A1	836	CLA	CED-O2D-CGD	2.24	121.12	115.97
16	B3	1847	BCR	C40-C30-C25	2.24	113.94	110.31
14	B1	821	CLA	C3C-C4C-NC	2.24	113.20	110.43
14	B5	1824	CLA	C3C-C4C-NC	2.24	113.20	110.43
14	A6	1619	CLA	C3B-C4B-NB	2.24	112.10	109.21
16	A1	845	BCR	C37-C22-C23	2.24	121.66	118.10
14	B3	1804	CLA	CMC-C2C-C1C	2.24	128.48	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A2	1621	CLA	CAC-C3C-C4C	2.24	127.91	124.82
14	F4	202	CLA	CED-O2D-CGD	2.24	121.13	115.97
14	A3	828	CLA	CED-O2D-CGD	2.24	121.13	115.97
16	A2	1649	BCR	C40-C30-C25	2.24	113.94	110.31
14	B1	822	CLA	C3C-C4C-NC	2.24	113.20	110.43
14	B6	831	CLA	C3C-C4C-NC	2.24	113.20	110.43
14	B2	811	CLA	CAC-C3C-C4C	2.24	127.91	124.82
14	A2	1616	CLA	CAC-C3C-C4C	2.24	127.91	124.82
16	J4	103	BCR	C33-C5-C6	2.24	127.02	124.51
14	M6	1201	CLA	CMC-C2C-C1C	2.24	128.48	125.05
14	A6	1604	CLA	CMC-C2C-C1C	2.24	128.48	125.05
14	B5	1824	CLA	C3B-C4B-NB	2.24	112.11	109.21
14	A2	1604	CLA	CHB-C4A-NA	2.24	127.61	124.51
14	A1	826	CLA	C2C-C1C-NC	2.24	112.41	110.09
14	K5	101	CLA	CAC-C3C-C4C	2.24	127.91	124.82
14	B6	812	CLA	CAC-C3C-C4C	2.24	127.91	124.82
14	A5	814	CLA	CAC-C3C-C4C	2.24	127.91	124.82
14	A5	813	CLA	CAC-C3C-C4C	2.24	127.91	124.82
14	A4	841	CLA	CAC-C3C-C4C	2.24	127.91	124.82
16	I4	102	BCR	C38-C26-C25	2.24	127.02	124.51
14	B2	805	CLA	C3C-C4C-NC	2.24	113.21	110.43
14	A5	819	CLA	C3C-C4C-NC	2.24	113.21	110.43
14	A5	813	CLA	CMB-C2B-C3B	2.24	128.97	124.88
14	B2	826	CLA	CMB-C2B-C3B	2.24	128.97	124.88
14	A2	1603	CLA	CMC-C2C-C1C	2.24	128.49	125.05
14	K3	1401	CLA	CAC-C3C-C4C	2.24	127.91	124.82
14	B6	817	CLA	C3C-C4C-NC	2.24	113.21	110.43
14	B6	810	CLA	CAC-C3C-C4C	2.24	127.92	124.82
14	B5	1819	CLA	CHB-C4A-NA	2.24	127.62	124.51
14	B6	807	CLA	C3B-C4B-NB	2.24	112.11	109.21
14	B1	813	CLA	C3C-C4C-NC	2.25	113.21	110.43
14	A2	1619	CLA	CMC-C2C-C1C	2.25	128.49	125.05
14	A3	810	CLA	CED-O2D-CGD	2.25	121.14	115.97
16	B4	846	BCR	C37-C22-C23	2.25	121.68	118.10
14	A4	812	CLA	CMB-C2B-C3B	2.25	128.97	124.88
14	B5	1804	CLA	CMB-C2B-C3B	2.25	128.97	124.88
14	A3	836	CLA	CMC-C2C-C1C	2.25	128.49	125.05
16	B3	1847	BCR	C36-C18-C19	2.25	121.68	118.10
14	X6	1701	CLA	C4A-NA-C1A	2.25	109.22	106.32
14	A6	1612	CLA	C4A-NA-C1A	2.25	109.22	106.32
14	A1	812	CLA	CMB-C2B-C3B	2.25	128.97	124.88
16	A6	1648	BCR	C34-C9-C8	2.25	121.68	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B1	844	BCR	C36-C18-C19	2.25	121.68	118.10
14	A4	805	CLA	C3C-C4C-NC	2.25	113.21	110.43
14	A3	832	CLA	CMC-C2C-C1C	2.25	128.50	125.05
14	B4	802	CLA	CHB-C4A-NA	2.25	127.62	124.51
14	B5	1801	CLA	CMB-C2B-C3B	2.25	128.98	124.88
14	A5	823	CLA	CAC-C3C-C4C	2.25	127.92	124.82
14	A3	837	CLA	C4A-NA-C1A	2.25	109.22	106.32
14	A4	815	CLA	CMC-C2C-C1C	2.25	128.50	125.05
14	A3	812	CLA	C4A-NA-C1A	2.25	109.22	106.32
14	L2	205	CLA	CMC-C2C-C1C	2.25	128.50	125.05
14	X3	102	CLA	CMC-C2C-C1C	2.25	128.50	125.05
14	A4	820	CLA	CAC-C3C-C4C	2.25	127.92	124.82
14	A4	834	CLA	CED-O2D-CGD	2.25	121.16	115.97
14	A2	1602	CLA	OBD-CAD-C3D	2.25	132.19	128.09
14	A6	1610	CLA	CED-O2D-CGD	2.25	121.16	115.97
14	A4	802	CLA	CMC-C2C-C1C	2.25	128.50	125.05
14	B4	808	CLA	C3C-C4C-NC	2.25	113.22	110.43
16	B2	843	BCR	C36-C18-C19	2.25	121.69	118.10
14	A6	1622	CLA	C2C-C1C-NC	2.25	112.42	110.09
16	F1	1302	BCR	C40-C30-C25	2.25	113.96	110.31
14	B3	1830	CLA	CAC-C3C-C4C	2.25	127.93	124.82
14	B4	832	CLA	CMC-C2C-C1C	2.25	128.50	125.05
14	B6	828	CLA	CMC-C2C-C1C	2.25	128.50	125.05
14	B3	1833	CLA	CED-O2D-CGD	2.25	121.17	115.97
14	A4	809	CLA	CED-O2D-CGD	2.25	121.17	115.97
14	B1	808	CLA	CMB-C2B-C3B	2.26	128.99	124.88
14	B1	813	CLA	CAC-C3C-C4C	2.26	127.93	124.82
14	B2	827	CLA	CMC-C2C-C1C	2.26	128.51	125.05
14	B3	1808	CLA	C3B-C4B-NB	2.26	112.13	109.21
14	A6	1606	CLA	C3C-C4C-NC	2.26	113.22	110.43
14	L6	207	CLA	C3C-C4C-NC	2.26	113.22	110.43
14	X5	101	CLA	CMC-C2C-C1C	2.26	128.51	125.05
16	L3	206	BCR	C29-C30-C25	2.26	114.00	110.48
14	A6	1608	CLA	C2C-C1C-NC	2.26	112.43	110.09
14	A2	1634	CLA	CMC-C2C-C1C	2.26	128.51	125.05
14	A4	814	CLA	C3C-C4C-NC	2.26	113.22	110.43
14	B5	1836	CLA	CHB-C4A-NA	2.26	127.63	124.51
16	A3	849	BCR	C40-C30-C25	2.26	113.97	110.31
14	A3	845	CLA	C2C-C1C-NC	2.26	112.43	110.09
14	A6	1627	CLA	C2C-C1C-NC	2.26	112.43	110.09
14	B1	838	CLA	O2A-CGA-CBA	2.26	118.45	111.92
14	A6	1651	CLA	CMC-C2C-C1C	2.26	128.51	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	807	CLA	CMB-C2B-C3B	2.26	128.99	124.88
16	B2	845	BCR	C38-C26-C25	2.26	127.04	124.51
14	B3	1802	CLA	C3C-C4C-NC	2.26	113.23	110.43
14	A2	1623	CLA	C3C-C4C-NC	2.26	113.23	110.43
14	B2	805	CLA	C3B-C4B-NB	2.26	112.13	109.21
14	K3	1401	CLA	CMC-C2C-C1C	2.26	128.51	125.05
16	A6	1644	BCR	C38-C26-C25	2.26	127.04	124.51
14	A2	1615	CLA	CMB-C2B-C3B	2.26	129.00	124.88
16	B6	844	BCR	C36-C18-C19	2.26	121.70	118.10
16	B5	1847	BCR	C36-C18-C19	2.26	121.70	118.10
14	A2	1636	CLA	C3C-C4C-NC	2.26	113.23	110.43
14	B5	1814	CLA	CED-O2D-CGD	2.26	121.18	115.97
16	B5	1850	BCR	C35-C13-C12	2.26	121.70	118.10
16	A2	1650	BCR	C37-C22-C23	2.26	121.70	118.10
14	B6	822	CLA	C3C-C4C-NC	2.26	113.23	110.43
14	F5	1301	CLA	CED-O2D-CGD	2.26	121.19	115.97
14	A5	834	CLA	C3C-C4C-NC	2.26	113.23	110.43
14	A3	821	CLA	C3C-C4C-NC	2.26	113.23	110.43
14	A4	835	CLA	C4A-NA-C1A	2.26	109.24	106.32
16	J1	103	BCR	C1-C6-C7	2.26	122.09	115.73
14	B4	830	CLA	CMC-C2C-C1C	2.26	128.52	125.05
14	A1	814	CLA	C4A-NA-C1A	2.26	109.24	106.32
16	B6	850	BCR	C37-C22-C23	2.26	121.71	118.10
14	B6	818	CLA	C3C-C4C-NC	2.27	113.23	110.43
14	B4	823	CLA	C4A-NA-C1A	2.27	109.24	106.32
16	A4	847	BCR	C33-C5-C6	2.27	127.04	124.51
14	A6	1628	CLA	CED-O2D-CGD	2.27	121.19	115.97
14	B5	1802	CLA	CHB-C4A-NA	2.27	127.65	124.51
14	B2	816	CLA	CHB-C4A-NA	2.27	127.65	124.51
14	L1	201	CLA	CMC-C2C-C1C	2.27	128.52	125.05
14	B2	827	CLA	CED-O2D-CGD	2.27	121.19	115.97
14	B5	1812	CLA	CAA-C2A-C1A	2.27	119.41	111.97
14	L6	206	CLA	CMC-C2C-C1C	2.27	128.53	125.05
14	A5	811	CLA	CED-O2D-CGD	2.27	121.20	115.97
14	A5	820	CLA	C2C-C1C-NC	2.27	112.44	110.09
14	B6	821	CLA	C2C-C1C-NC	2.27	112.44	110.09
14	A1	819	CLA	C2C-C1C-NC	2.27	112.44	110.09
14	B1	806	CLA	C3C-C4C-NC	2.27	113.24	110.43
14	A1	815	CLA	CMC-C2C-C1C	2.27	128.53	125.05
14	A2	1610	CLA	C2C-C1C-NC	2.27	112.44	110.09
14	A6	1613	CLA	C3C-C4C-NC	2.27	113.24	110.43
14	B4	835	CLA	C3C-C4C-NC	2.27	113.24	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	806	CLA	CAC-C3C-C4C	2.27	127.95	124.82
16	B2	844	BCR	C36-C18-C19	2.27	121.72	118.10
16	B1	847	BCR	C29-C30-C25	2.27	114.03	110.48
14	A1	814	CLA	C3B-C4B-NB	2.27	112.15	109.21
14	L6	203	CLA	CED-O2D-CGD	2.27	121.20	115.97
17	A5	852	LHG	O2-C2-C3	2.27	117.68	109.42
14	A4	833	CLA	C3C-C4C-NC	2.27	113.24	110.43
14	A5	813	CLA	C3C-C4C-NC	2.27	113.24	110.43
14	B3	1824	CLA	C3B-C4B-NB	2.27	112.15	109.21
14	A3	816	CLA	CED-O2D-CGD	2.27	121.21	115.97
14	A5	807	CLA	CED-O2D-CGD	2.27	121.21	115.97
14	A2	1618	CLA	CMC-C2C-C1C	2.27	128.53	125.05
16	B1	849	BCR	C33-C5-C6	2.27	127.05	124.51
14	A2	1617	CLA	C3C-C4C-NC	2.27	113.25	110.43
14	F2	204	CLA	C3C-C4C-NC	2.27	113.25	110.43
16	A1	847	BCR	C34-C9-C8	2.27	121.72	118.10
14	A4	817	CLA	CED-O2D-CGD	2.27	121.21	115.97
16	J6	1104	BCR	C1-C6-C7	2.28	122.12	115.73
14	L4	203	CLA	CMC-C2C-C1C	2.28	128.54	125.05
16	M4	101	BCR	C33-C5-C6	2.28	127.06	124.51
16	A5	848	BCR	C33-C5-C6	2.28	127.06	124.51
14	B5	1826	CLA	C4-C3-C5	2.28	119.21	115.29
14	A5	807	CLA	CMC-C2C-C1C	2.28	128.54	125.05
14	B4	811	CLA	C3B-C4B-NB	2.28	112.15	109.21
14	J5	101	CLA	C4A-NA-C1A	2.28	109.26	106.32
14	B1	808	CLA	C3B-C4B-NB	2.28	112.16	109.21
14	A6	1619	CLA	C3C-C4C-NC	2.28	113.25	110.43
14	A3	831	CLA	CMC-C2C-C1C	2.28	128.54	125.05
14	B2	822	CLA	CMC-C2C-C1C	2.28	128.54	125.05
14	A3	828	CLA	C3B-C4B-NB	2.28	112.16	109.21
14	B5	1825	CLA	C3C-C4C-NC	2.28	113.25	110.43
14	B2	823	CLA	CED-O2D-CGD	2.28	121.22	115.97
14	A5	816	CLA	CED-O2D-CGD	2.28	121.22	115.97
14	A5	819	CLA	CED-O2D-CGD	2.28	121.22	115.97
14	B6	804	CLA	CED-O2D-CGD	2.28	121.22	115.97
14	A6	1615	CLA	C4A-NA-C1A	2.28	109.26	106.32
14	A6	1615	CLA	C3C-C4C-NC	2.28	113.25	110.43
16	I4	102	BCR	C30-C25-C24	2.28	122.14	115.73
16	A4	845	BCR	C38-C26-C25	2.28	127.06	124.51
14	A5	821	CLA	CAC-C3C-C4C	2.28	127.97	124.82
14	J6	1103	CLA	C3C-C4C-NC	2.28	113.25	110.43
14	L5	206	CLA	CAC-C3C-C4C	2.28	127.97	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	823	CLA	C3B-C4B-NB	2.28	112.16	109.21
14	A1	805	CLA	C3C-C4C-NC	2.28	113.25	110.43
14	B3	1805	CLA	C3C-C4C-NC	2.28	113.25	110.43
14	A2	1633	CLA	CMC-C2C-C1C	2.28	128.55	125.05
14	B1	828	CLA	CMB-C2B-C3B	2.28	129.04	124.88
14	A3	831	CLA	C2C-C1C-NC	2.28	112.45	110.09
14	A2	1643	CLA	CMB-C2B-C3B	2.28	129.04	124.88
17	A4	851	LHG	O2-C2-C3	2.28	117.73	109.42
14	A3	819	CLA	C3C-C4C-NC	2.28	113.26	110.43
14	A5	806	CLA	CAC-C3C-C4C	2.28	127.97	124.82
16	B1	852	BCR	C37-C22-C23	2.28	121.74	118.10
14	B3	1833	CLA	C3C-C4C-NC	2.28	113.26	110.43
14	A5	815	CLA	C4A-NA-C1A	2.28	109.27	106.32
14	B4	817	CLA	CMC-C2C-C1C	2.28	128.55	125.05
14	A5	808	CLA	C2C-C1C-NC	2.29	112.46	110.09
14	A5	843	CLA	C2C-C1C-NC	2.29	112.46	110.09
16	B1	847	BCR	C36-C18-C19	2.29	121.74	118.10
14	B3	1836	CLA	CHB-C4A-NA	2.29	127.67	124.51
16	A3	848	BCR	C38-C26-C25	2.29	127.07	124.51
14	B1	822	CLA	C4A-NA-C1A	2.29	109.27	106.32
16	J1	103	BCR	C35-C13-C12	2.29	121.74	118.10
14	A5	816	CLA	CMC-C2C-C1C	2.29	128.55	125.05
14	B5	1808	CLA	C3C-C4C-NC	2.29	113.26	110.43
14	B3	1808	CLA	CMB-C2B-C3B	2.29	129.04	124.88
16	A6	1646	BCR	C37-C22-C23	2.29	121.74	118.10
14	A5	835	CLA	CMC-C2C-C1C	2.29	128.56	125.05
16	L4	206	BCR	C37-C22-C23	2.29	121.74	118.10
14	B4	819	CLA	C3C-C4C-NC	2.29	113.26	110.43
16	B4	847	BCR	C36-C18-C19	2.29	121.75	118.10
14	B2	820	CLA	C2C-C1C-NC	2.29	112.46	110.09
14	A1	836	CLA	CAC-C3C-C4C	2.29	127.98	124.82
14	A3	819	CLA	CAC-C3C-C4C	2.29	127.98	124.82
14	A3	815	CLA	C3C-C4C-NC	2.29	113.27	110.43
14	A4	820	CLA	C3C-C4C-NC	2.29	113.27	110.43
14	B4	815	CLA	C3B-C4B-NB	2.29	112.17	109.21
16	A3	850	BCR	C37-C22-C23	2.29	121.75	118.10
14	A3	822	CLA	C2C-C1C-NC	2.29	112.46	110.09
14	A2	1604	CLA	C3C-C4C-NC	2.29	113.27	110.43
14	B1	807	CLA	C3C-C4C-NC	2.29	113.27	110.43
14	B3	1823	CLA	C3C-C4C-NC	2.29	113.27	110.43
14	A4	825	CLA	C3B-C4B-NB	2.29	112.17	109.21
16	A5	853	BCR	C33-C5-C6	2.29	127.07	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A6	1645	BCR	C40-C30-C25	2.29	114.03	110.31
14	B5	1830	CLA	CAC-C3C-C4C	2.29	127.98	124.82
14	A4	832	CLA	C3C-C4C-NC	2.29	113.27	110.43
14	A6	1630	CLA	CMC-C2C-C1C	2.30	128.57	125.05
16	L6	209	BCR	C38-C26-C25	2.30	127.08	124.51
14	L4	205	CLA	CAC-C3C-C4C	2.30	127.99	124.82
14	B4	818	CLA	CED-O2D-CGD	2.30	121.27	115.97
14	B4	814	CLA	CAC-C3C-C4C	2.30	127.99	124.82
14	A4	835	CLA	CAC-C3C-C4C	2.30	127.99	124.82
14	K5	102	CLA	CAC-C3C-C4C	2.30	127.99	124.82
14	B3	1820	CLA	C3C-C4C-NC	2.30	113.28	110.43
14	B4	827	CLA	C3C-C4C-NC	2.30	113.28	110.43
14	B3	1824	CLA	CED-O2D-CGD	2.30	121.27	115.97
16	L1	203	BCR	C30-C25-C24	2.30	122.19	115.73
14	B5	1834	CLA	C11-C10-C8	2.30	123.29	115.73
14	B6	831	CLA	C2C-C1C-NC	2.30	112.47	110.09
14	B1	829	CLA	CAC-C3C-C4C	2.30	127.99	124.82
14	B6	815	CLA	CMC-C2C-C1C	2.30	128.58	125.05
14	X2	1701	CLA	C4A-NA-C1A	2.30	109.29	106.32
14	B4	837	CLA	CMB-C2B-C3B	2.30	129.07	124.88
14	A2	1640	CLA	CED-O2D-CGD	2.30	121.28	115.97
14	A5	824	CLA	CAC-C3C-C4C	2.30	128.00	124.82
14	A2	1629	CLA	C2C-C1C-NC	2.30	112.47	110.09
14	A2	1637	CLA	CMC-C2C-C1C	2.30	128.58	125.05
16	A3	856	BCR	C34-C9-C8	2.30	121.77	118.10
14	A3	808	CLA	C2C-C1C-NC	2.30	112.47	110.09
14	A6	1632	CLA	C3C-C4C-NC	2.30	113.28	110.43
14	A1	813	CLA	C3C-C4C-NC	2.30	113.28	110.43
14	A4	834	CLA	CMC-C2C-C1C	2.30	128.58	125.05
14	B3	1816	CLA	CED-O2D-CGD	2.30	121.28	115.97
16	J6	1105	BCR	C36-C18-C19	2.30	121.77	118.10
14	B2	820	CLA	C4A-NA-C1A	2.30	109.30	106.32
16	L2	203	BCR	C30-C25-C24	2.31	122.21	115.73
14	A2	1607	CLA	CED-O2D-CGD	2.31	121.28	115.97
14	L3	203	CLA	CMC-C2C-C1C	2.31	128.58	125.05
14	M2	1201	CLA	CMC-C2C-C1C	2.31	128.58	125.05
14	A1	818	CLA	C3B-C4B-NB	2.31	112.19	109.21
14	A3	815	CLA	C4A-NA-C1A	2.31	109.30	106.32
14	A3	820	CLA	C2C-C1C-NC	2.31	112.48	110.09
14	A6	1604	CLA	CMB-C2B-C3B	2.31	129.08	124.88
14	A4	812	CLA	CED-O2D-CGD	2.31	121.29	115.97
14	B1	824	CLA	CAC-C3C-C4C	2.31	128.00	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1625	CLA	CMC-C2C-C1C	2.31	128.59	125.05
16	J3	103	BCR	C1-C6-C7	2.31	122.22	115.73
16	L6	204	BCR	C30-C25-C24	2.31	122.22	115.73
14	B1	801	CLA	CMB-C2B-C3B	2.31	129.08	124.88
14	B3	1815	CLA	C3B-C4B-NB	2.31	112.19	109.21
14	B1	832	CLA	CED-O2D-CGD	2.31	121.29	115.97
14	A2	1624	CLA	C2C-C1C-NC	2.31	112.48	110.09
14	A5	809	CLA	CMB-C2B-C3B	2.31	129.09	124.88
14	A6	1640	CLA	CED-O2D-CGD	2.31	121.29	115.97
14	B2	828	CLA	CMC-C2C-C1C	2.31	128.59	125.05
14	B6	825	CLA	C3C-C4C-NC	2.31	113.29	110.43
14	A3	813	CLA	C3C-C4C-NC	2.31	113.29	110.43
14	A3	826	CLA	C3B-C4B-NB	2.31	112.20	109.21
16	I2	101	BCR	C38-C26-C25	2.31	127.10	124.51
16	B6	845	BCR	C36-C18-C19	2.31	121.78	118.10
14	A3	835	CLA	C3C-C4C-NC	2.31	113.29	110.43
16	J1	103	BCR	C33-C5-C6	2.31	127.10	124.51
14	B4	826	CLA	CED-O2D-CGD	2.31	121.30	115.97
14	B5	1826	CLA	C2C-C1C-NC	2.31	112.49	110.09
14	A1	820	CLA	O2A-CGA-CBA	2.31	118.61	111.92
14	A1	817	CLA	CED-O2D-CGD	2.31	121.30	115.97
14	B2	808	CLA	C3B-C4B-NB	2.32	112.20	109.21
16	J5	103	BCR	C1-C6-C7	2.32	122.24	115.73
14	A2	1627	CLA	CMC-C2C-C1C	2.32	128.60	125.05
16	A2	1649	BCR	C38-C26-C25	2.32	127.10	124.51
14	J5	101	CLA	C3C-C4C-NC	2.32	113.30	110.43
14	B4	823	CLA	C2C-C1C-NC	2.32	112.49	110.09
16	A2	1648	BCR	C38-C26-C25	2.32	127.10	124.51
16	B2	847	BCR	C33-C5-C6	2.32	127.10	124.51
14	L1	207	CLA	CAC-C3C-C4C	2.32	128.01	124.82
16	F4	201	BCR	C38-C26-C25	2.32	127.10	124.51
14	A4	814	CLA	C3B-C4B-NB	2.32	112.21	109.21
14	A1	824	CLA	C9-C8-C10	2.32	119.79	111.36
14	A4	840	CLA	CED-O2D-CGD	2.32	121.31	115.97
14	A5	806	CLA	C3C-C4C-NC	2.32	113.30	110.43
14	B2	833	CLA	CHB-C4A-NA	2.32	127.72	124.51
16	B4	846	BCR	C33-C5-C6	2.32	127.10	124.51
14	A6	1638	CLA	CED-O2D-CGD	2.32	121.31	115.97
14	B6	820	CLA	CED-O2D-CGD	2.32	121.31	115.97
16	J2	102	BCR	C1-C6-C7	2.32	122.25	115.73
14	B3	1824	CLA	C1-O2A-CGA	2.32	122.12	116.77
14	A3	837	CLA	CAC-C3C-C4C	2.32	128.02	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1613	CLA	CAC-C3C-C4C	2.32	128.02	124.82
14	A3	818	CLA	CED-O2D-CGD	2.32	121.32	115.97
14	A4	831	CLA	CED-O2D-CGD	2.32	121.32	115.97
14	A6	1651	CLA	CMB-C2B-C3B	2.32	129.11	124.88
14	B4	812	CLA	C3C-C4C-NC	2.32	113.30	110.43
14	A2	1611	CLA	CMB-C2B-C3B	2.32	129.11	124.88
14	J2	101	CLA	C3C-C4C-NC	2.32	113.30	110.43
16	I3	102	BCR	C32-C1-C6	2.32	114.08	110.31
16	J3	103	BCR	C35-C13-C12	2.32	121.80	118.10
14	B5	1803	CLA	O2D-CGD-CBD	2.32	115.40	111.28
14	A4	821	CLA	C2C-C1C-NC	2.32	112.50	110.09
14	B5	1801	CLA	C2C-C1C-NC	2.32	112.50	110.09
14	B2	830	CLA	C3C-C4C-NC	2.32	113.31	110.43
16	F2	201	BCR	C36-C18-C19	2.32	121.80	118.10
14	A5	806	CLA	O2D-CGD-CBD	2.32	115.41	111.28
14	A1	839	CLA	CAC-C3C-C4C	2.32	128.03	124.82
14	A2	1630	CLA	C3B-C4B-NB	2.33	112.22	109.21
14	A2	1643	CLA	C2C-C1C-NC	2.33	112.50	110.09
14	B1	826	CLA	C3C-C4C-NC	2.33	113.31	110.43
14	A3	805	CLA	CED-O2D-CGD	2.33	121.33	115.97
14	A4	805	CLA	CED-O2D-CGD	2.33	121.33	115.97
14	B3	1830	CLA	CMC-C2C-C1C	2.33	128.62	125.05
14	A2	1635	CLA	C3C-C4C-NC	2.33	113.31	110.43
16	A5	850	BCR	C34-C9-C8	2.33	121.81	118.10
14	A3	843	CLA	CAC-C3C-C4C	2.33	128.03	124.82
14	B6	833	CLA	CED-O2D-CGD	2.33	121.34	115.97
14	B3	1802	CLA	CHB-C4A-NA	2.33	127.73	124.51
14	A2	1620	CLA	CED-O2D-CGD	2.33	121.34	115.97
14	A4	830	CLA	CMC-C2C-C1C	2.33	128.62	125.05
14	B5	1831	CLA	C3C-C4C-NC	2.33	113.31	110.43
16	M3	1602	BCR	C33-C5-C6	2.33	127.12	124.51
14	B5	1823	CLA	C2C-C1C-NC	2.33	112.50	110.09
14	B2	816	CLA	CED-O2D-CGD	2.33	121.34	115.97
16	A1	845	BCR	C33-C5-C6	2.33	127.12	124.51
14	A4	827	CLA	C3B-C4B-NB	2.33	112.23	109.21
14	B6	834	CLA	CHB-C4A-NA	2.33	127.74	124.51
14	K5	101	CLA	C3C-C4C-NC	2.33	113.32	110.43
14	B2	834	CLA	CMB-C2B-C3B	2.33	129.13	124.88
14	A1	805	CLA	O2D-CGD-CBD	2.33	115.42	111.28
14	A4	831	CLA	CMC-C2C-C1C	2.33	128.63	125.05
16	B1	848	BCR	C36-C18-C19	2.33	121.82	118.10
16	B1	852	BCR	C8-C7-C6	2.33	133.79	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A4	846	BCR	C37-C22-C23	2.33	121.82	118.10
14	B2	832	CLA	C3C-C4C-NC	2.33	113.32	110.43
14	A2	1638	CLA	CAC-C3C-C4C	2.34	128.04	124.82
14	A5	822	CLA	C2C-C1C-NC	2.34	112.51	110.09
14	A2	1628	CLA	C3B-C4B-NB	2.34	112.23	109.21
16	B1	845	BCR	C38-C26-C25	2.34	127.12	124.51
14	X2	1701	CLA	C3C-C4C-NC	2.34	113.32	110.43
14	B5	1830	CLA	CMC-C2C-C1C	2.34	128.63	125.05
14	B3	1814	CLA	CAC-C3C-C4C	2.34	128.04	124.82
14	A5	814	CLA	CED-O2D-CGD	2.34	121.36	115.97
14	A2	1612	CLA	CED-O2D-CGD	2.34	121.36	115.97
14	A1	808	CLA	CMB-C2B-C3B	2.34	129.14	124.88
14	B1	853	CLA	C1-C2-C3	2.34	130.26	125.96
16	B2	847	BCR	C34-C9-C8	2.34	121.82	118.10
16	L3	206	BCR	C37-C22-C23	2.34	121.82	118.10
16	J4	103	BCR	C35-C13-C12	2.34	121.82	118.10
14	B4	814	CLA	C4A-NA-C1A	2.34	109.34	106.32
14	B6	817	CLA	CHB-C4A-NA	2.34	127.75	124.51
14	A4	812	CLA	CAC-C3C-C4C	2.34	128.04	124.82
14	A6	1636	CLA	CAC-C3C-C4C	2.34	128.04	124.82
14	B2	823	CLA	C2C-C1C-NC	2.34	112.51	110.09
14	B6	809	CLA	CMC-C2C-C1C	2.34	128.63	125.05
16	M3	1602	BCR	C32-C1-C6	2.34	114.10	110.31
14	B2	809	CLA	C3B-C4B-NB	2.34	112.23	109.21
14	A2	1617	CLA	C4A-NA-C1A	2.34	109.34	106.32
14	L6	208	CLA	CAC-C3C-C4C	2.34	128.05	124.82
14	B4	823	CLA	CED-O2D-CGD	2.34	121.36	115.97
16	B1	844	BCR	C33-C5-C6	2.34	127.13	124.51
16	A4	847	BCR	C37-C22-C23	2.34	121.83	118.10
16	L2	208	BCR	C38-C26-C25	2.34	127.13	124.51
14	A3	840	CLA	C2C-C1C-NC	2.34	112.51	110.09
14	M1	1201	CLA	CMC-C2C-C1C	2.34	128.64	125.05
14	A2	1626	CLA	CAC-C3C-C4C	2.34	128.05	124.82
14	A1	823	CLA	C3C-C4C-NC	2.34	113.33	110.43
14	B5	1835	CLA	C4A-NA-C1A	2.34	109.34	106.32
16	J2	102	BCR	C33-C5-C6	2.34	127.13	124.51
14	B3	1826	CLA	C4-C3-C5	2.34	119.33	115.29
14	A6	1640	CLA	C1-O2A-CGA	2.34	122.17	116.77
14	A4	826	CLA	C2C-C1C-NC	2.34	112.52	110.09
14	A6	1614	CLA	CED-O2D-CGD	2.34	121.37	115.97
14	B1	833	CLA	C3C-C4C-NC	2.34	113.33	110.43
14	B3	1801	CLA	C2C-C1C-NC	2.34	112.52	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	827	CLA	C11-C10-C8	2.34	123.43	115.73
14	B1	802	CLA	CHB-C4A-NA	2.35	127.75	124.51
14	A3	819	CLA	C3B-C4B-NB	2.35	112.24	109.21
14	B1	813	CLA	C4A-NA-C1A	2.35	109.35	106.32
14	A3	824	CLA	C3C-C4C-NC	2.35	113.33	110.43
14	B6	824	CLA	CMC-C2C-C1C	2.35	128.65	125.05
16	I5	102	BCR	C30-C25-C24	2.35	122.33	115.73
14	A1	807	CLA	C2C-C1C-NC	2.35	112.52	110.09
14	X6	1701	CLA	CMC-C2C-C1C	2.35	128.65	125.05
14	B5	1834	CLA	C3C-C4C-NC	2.35	113.33	110.43
14	A4	816	CLA	CED-O2D-CGD	2.35	121.38	115.97
14	A4	810	CLA	CED-O2D-CGD	2.35	121.38	115.97
14	B3	1835	CLA	C3C-C4C-NC	2.35	113.34	110.43
14	A6	1628	CLA	C3B-C4B-NB	2.35	112.25	109.21
14	B4	805	CLA	C11-C10-C8	2.35	123.44	115.73
14	B3	1837	CLA	CED-O2D-CGD	2.35	121.38	115.97
16	I3	102	BCR	C30-C25-C24	2.35	122.33	115.73
16	M6	1202	BCR	C32-C1-C6	2.35	114.12	110.31
14	B3	1821	CLA	CED-O2D-CGD	2.35	121.38	115.97
14	B4	808	CLA	C3B-C4B-NB	2.35	112.25	109.21
14	B6	824	CLA	C3C-C4C-NC	2.35	113.34	110.43
14	A6	1634	CLA	C3C-C4C-NC	2.35	113.34	110.43
14	B2	829	CLA	CMC-C2C-C1C	2.35	128.65	125.05
14	A3	816	CLA	CMC-C2C-C1C	2.35	128.65	125.05
14	B3	1811	CLA	CMC-C2C-C1C	2.35	128.65	125.05
16	A6	1652	BCR	C34-C9-C8	2.35	121.84	118.10
14	B6	819	CLA	CED-O2D-CGD	2.35	121.38	115.97
14	A5	814	CLA	C3C-C4C-NC	2.35	113.34	110.43
14	B3	1816	CLA	C3C-C4C-NC	2.35	113.34	110.43
14	B6	829	CLA	CMC-C2C-C1C	2.35	128.65	125.05
14	B5	1827	CLA	C3C-C4C-NC	2.35	113.34	110.43
16	A5	848	BCR	C37-C22-C23	2.35	121.84	118.10
14	B2	834	CLA	CED-O2D-CGD	2.35	121.39	115.97
16	L1	203	BCR	C2-C1-C6	2.35	114.15	110.48
16	I5	102	BCR	C36-C18-C19	2.35	121.85	118.10
14	A6	1613	CLA	CED-O2D-CGD	2.35	121.39	115.97
14	A5	815	CLA	C3C-C4C-NC	2.35	113.34	110.43
14	B4	805	CLA	C3C-C4C-NC	2.35	113.34	110.43
14	A3	804	CLA	CMB-C2B-C3B	2.35	129.16	124.88
14	B4	830	CLA	CED-O2D-CGD	2.35	121.39	115.97
14	B5	1809	CLA	CED-O2D-CGD	2.35	121.39	115.97
16	J5	105	BCR	C8-C7-C6	2.35	133.84	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A2	1649	BCR	C37-C22-C23	2.35	121.85	118.10
14	B4	816	CLA	C3C-C4C-NC	2.35	113.34	110.43
14	A4	812	CLA	C3C-C4C-NC	2.35	113.34	110.43
14	B2	837	CLA	C2C-C1C-NC	2.35	112.53	110.09
14	A4	813	CLA	C3C-C4C-NC	2.36	113.34	110.43
16	B5	1846	BCR	C33-C5-C6	2.36	127.14	124.51
14	B2	802	CLA	CMC-C2C-C1C	2.36	128.66	125.05
14	A4	808	CLA	CMB-C2B-C3B	2.36	129.17	124.88
14	B4	826	CLA	C3C-C4C-NC	2.36	113.35	110.43
14	B5	1819	CLA	C3C-C4C-NC	2.36	113.35	110.43
14	A6	1605	CLA	CED-O2D-CGD	2.36	121.40	115.97
14	A6	1609	CLA	CMC-C2C-C1C	2.36	128.66	125.05
14	B5	1817	CLA	CMC-C2C-C1C	2.36	128.66	125.05
14	B1	818	CLA	CMB-C2B-C3B	2.36	129.17	124.88
14	B5	1808	CLA	CMB-C2B-C3B	2.36	129.17	124.88
14	A4	801	CLA	OBD-CAD-C3D	2.36	132.38	128.09
14	A3	833	CLA	C3C-C4C-NC	2.36	113.35	110.43
14	A1	832	CLA	C3C-C4C-NC	2.36	113.35	110.43
14	A4	804	CLA	CED-O2D-CGD	2.36	121.40	115.97
14	A3	814	CLA	CED-O2D-CGD	2.36	121.40	115.97
14	B1	829	CLA	CED-O2D-CGD	2.36	121.40	115.97
14	B6	838	CLA	C2C-C1C-NC	2.36	112.53	110.09
14	A1	821	CLA	C2C-C1C-NC	2.36	112.53	110.09
14	A6	1639	CLA	CAC-C3C-C4C	2.36	128.07	124.82
14	B4	805	CLA	CED-O2D-CGD	2.36	121.41	115.97
14	B5	1822	CLA	CED-O2D-CGD	2.36	121.41	115.97
14	B6	805	CLA	CED-O2D-CGD	2.36	121.41	115.97
16	B1	848	BCR	C38-C26-C25	2.36	127.15	124.51
16	M2	1202	BCR	C32-C1-C6	2.36	114.14	110.31
14	A3	836	CLA	CED-O2D-CGD	2.36	121.41	115.97
14	B4	821	CLA	CED-O2D-CGD	2.36	121.41	115.97
14	B3	1809	CLA	CED-O2D-CGD	2.36	121.41	115.97
14	B4	829	CLA	CMB-C2B-C3B	2.36	129.18	124.88
14	B2	805	CLA	CMB-C2B-C3B	2.36	129.18	124.88
14	A4	853	CLA	CED-O2D-CGD	2.36	121.41	115.97
14	A4	824	CLA	CMC-C2C-C1C	2.36	128.67	125.05
14	B1	816	CLA	CMC-C2C-C1C	2.36	128.67	125.05
14	B3	1827	CLA	C3C-C4C-NC	2.36	113.36	110.43
14	A2	1626	CLA	C3C-C4C-NC	2.36	113.36	110.43
14	A5	804	CLA	CMB-C2B-C3B	2.36	129.18	124.88
14	J3	101	CLA	C3C-C4C-NC	2.36	113.36	110.43
16	A1	847	BCR	C33-C5-C6	2.36	127.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	808	CLA	CMB-C2B-C3B	2.36	129.19	124.88
14	B2	813	CLA	C3C-C4C-NC	2.37	113.36	110.43
14	B2	817	CLA	C3C-C4C-NC	2.37	113.36	110.43
14	B6	833	CLA	C3C-C4C-NC	2.37	113.36	110.43
16	A3	856	BCR	C33-C5-C6	2.37	127.16	124.51
14	A6	1616	CLA	CMC-C2C-C1C	2.37	128.68	125.05
14	A1	839	CLA	C4-C3-C5	2.37	119.37	115.29
14	B2	821	CLA	CED-O2D-CGD	2.37	121.42	115.97
14	B1	819	CLA	C3B-C4B-NB	2.37	112.27	109.21
14	L6	202	CLA	CMC-C2C-C1C	2.37	128.68	125.05
16	A1	843	BCR	C38-C26-C25	2.37	127.16	124.51
16	B2	850	BCR	C8-C7-C6	2.37	133.88	127.25
14	A2	1613	CLA	CED-O2D-CGD	2.37	121.42	115.97
14	B1	824	CLA	C3C-C4C-NC	2.37	113.36	110.43
16	F4	204	BCR	C8-C7-C6	2.37	133.88	127.25
16	J4	103	BCR	C1-C6-C7	2.37	122.38	115.73
16	J5	103	BCR	C33-C5-C6	2.37	127.16	124.51
14	B4	820	CLA	C3B-C4B-NB	2.37	112.27	109.21
14	B1	803	CLA	C3C-C4C-NC	2.37	113.36	110.43
16	A3	856	BCR	C37-C22-C23	2.37	121.87	118.10
16	F6	201	BCR	C38-C26-C25	2.37	127.16	124.51
14	B6	815	CLA	CMB-C2B-C3B	2.37	129.20	124.88
16	F4	201	BCR	C35-C13-C12	2.37	121.88	118.10
16	B3	1851	BCR	C8-C7-C6	2.37	133.89	127.25
14	A2	1603	CLA	CED-O2D-CGD	2.37	121.44	115.97
14	B1	822	CLA	C2C-C1C-NC	2.37	112.55	110.09
16	J3	104	BCR	C32-C1-C6	2.37	114.16	110.31
14	B3	1808	CLA	C3C-C4C-NC	2.37	113.37	110.43
14	A1	809	CLA	CED-O2D-CGD	2.37	121.44	115.97
16	B5	1847	BCR	C38-C26-C25	2.37	127.17	124.51
14	B1	804	CLA	O2D-CGD-CBD	2.37	115.49	111.28
14	A4	853	CLA	C4A-NA-C1A	2.37	109.39	106.32
14	A1	826	CLA	C3C-C4C-NC	2.38	113.37	110.43
14	B5	1826	CLA	C3C-C4C-NC	2.38	113.37	110.43
16	A3	852	BCR	C34-C9-C8	2.38	121.88	118.10
14	J1	101	CLA	CED-O2D-CGD	2.38	121.44	115.97
14	B1	835	CLA	CHB-C4A-NA	2.38	127.80	124.51
14	A2	1640	CLA	C3C-C4C-NC	2.38	113.37	110.43
14	B1	818	CLA	C3C-C4C-NC	2.38	113.37	110.43
14	A1	827	CLA	C3B-C4B-NB	2.38	112.28	109.21
16	B1	848	BCR	C35-C13-C12	2.38	121.89	118.10
14	B5	1805	CLA	C3C-C4C-NC	2.38	113.37	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	805	CLA	C11-C10-C8	2.38	123.54	115.73
16	A6	1646	BCR	C30-C25-C24	2.38	122.41	115.73
16	B2	847	BCR	C37-C22-C23	2.38	121.89	118.10
14	A5	817	CLA	CED-O2D-CGD	2.38	121.45	115.97
14	B3	1842	CLA	O2A-CGA-CBA	2.38	118.80	111.92
14	A2	1603	CLA	O2A-CGA-CBA	2.38	118.80	111.92
14	B6	812	CLA	CED-O2D-CGD	2.38	121.45	115.97
14	A6	1635	CLA	CED-O2D-CGD	2.38	121.46	115.97
16	J6	1104	BCR	C35-C13-C12	2.38	121.89	118.10
14	B2	819	CLA	CED-O2D-CGD	2.38	121.46	115.97
14	A4	838	CLA	C3C-C4C-NC	2.38	113.38	110.43
14	A6	1614	CLA	C3C-C4C-NC	2.38	113.38	110.43
14	A3	814	CLA	C3C-C4C-NC	2.38	113.38	110.43
16	A1	847	BCR	C37-C22-C23	2.38	121.89	118.10
14	B3	1823	CLA	C4A-NA-C1A	2.38	109.39	106.32
14	B1	832	CLA	C2C-C1C-NC	2.38	112.56	110.09
14	B3	1823	CLA	C2C-C1C-NC	2.38	112.56	110.09
14	A6	1613	CLA	CMB-C2B-C3B	2.38	129.22	124.88
14	A4	807	CLA	C2C-C1C-NC	2.38	112.56	110.09
14	A2	1641	CLA	C3C-C4C-NC	2.38	113.38	110.43
14	B2	823	CLA	C3C-C4C-NC	2.38	113.38	110.43
16	A5	850	BCR	C1-C6-C7	2.38	122.43	115.73
14	B2	811	CLA	CED-O2D-CGD	2.38	121.46	115.97
14	B1	801	CLA	CED-O2D-CGD	2.39	121.47	115.97
17	A1	849	LHG	C25-C24-C23	2.39	126.02	114.17
14	A1	833	CLA	C3C-C4C-NC	2.39	113.38	110.43
14	B5	1824	CLA	C1-O2A-CGA	2.39	122.27	116.77
14	A5	842	CLA	C4-C3-C5	2.39	119.41	115.29
14	A4	837	CLA	C3C-C4C-NC	2.39	113.39	110.43
14	B6	812	CLA	C4A-NA-C1A	2.39	109.40	106.32
14	A5	813	CLA	CED-O2D-CGD	2.39	121.47	115.97
14	B1	829	CLA	CMC-C2C-C1C	2.39	128.71	125.05
14	A2	1641	CLA	C2C-C1C-NC	2.39	112.56	110.09
14	J3	102	CLA	C3C-C4C-NC	2.39	113.39	110.43
16	B4	850	BCR	C34-C9-C8	2.39	121.91	118.10
14	A4	818	CLA	C3B-C4B-NB	2.39	112.30	109.21
14	B4	812	CLA	C3B-C4B-NB	2.39	112.30	109.21
14	A3	824	CLA	CAC-C3C-C4C	2.39	128.12	124.82
16	A6	1652	BCR	C37-C22-C23	2.39	121.91	118.10
14	A6	1627	CLA	C3C-C4C-NC	2.39	113.39	110.43
14	A3	840	CLA	C3C-C4C-NC	2.39	113.39	110.43
14	B2	822	CLA	C3C-C4C-NC	2.39	113.39	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F2	201	BCR	C38-C26-C25	2.39	127.19	124.51
14	A5	830	CLA	O2A-CGA-CBA	2.39	118.84	111.92
14	X4	102	CLA	C3C-C4C-NC	2.39	113.39	110.43
14	B3	1822	CLA	CED-O2D-CGD	2.39	121.48	115.97
14	A2	1621	CLA	C3B-C4B-NB	2.39	112.30	109.21
14	A1	803	CLA	CMB-C2B-C3B	2.39	129.24	124.88
14	A6	1640	CLA	C2C-C1C-NC	2.39	112.57	110.09
14	A1	825	CLA	C3B-C4B-NB	2.39	112.31	109.21
14	B4	824	CLA	C3B-C4B-NB	2.39	112.31	109.21
14	A5	810	CLA	CED-O2D-CGD	2.39	121.49	115.97
14	B4	824	CLA	CED-O2D-CGD	2.39	121.49	115.97
16	F3	201	BCR	C38-C26-C25	2.39	127.19	124.51
16	A2	1652	BCR	C33-C5-C6	2.39	127.19	124.51
14	X4	102	CLA	C4A-NA-C1A	2.39	109.41	106.32
14	A2	1608	CLA	CED-O2D-CGD	2.40	121.49	115.97
14	B4	836	CLA	CHB-C4A-NA	2.40	127.83	124.51
16	J3	104	BCR	C36-C18-C19	2.40	121.92	118.10
14	J6	1102	CLA	C3C-C4C-NC	2.40	113.40	110.43
14	B5	1826	CLA	CED-O2D-CGD	2.40	121.49	115.97
14	X5	101	CLA	C3C-C4C-NC	2.40	113.40	110.43
14	A3	839	CLA	CED-O2D-CGD	2.40	121.50	115.97
16	J2	103	BCR	C36-C18-C19	2.40	121.92	118.10
14	L6	202	CLA	CED-O2D-CGD	2.40	121.50	115.97
16	I4	102	BCR	C36-C18-C19	2.40	121.92	118.10
14	B2	810	CLA	C3C-C4C-NC	2.40	113.40	110.43
14	A2	1637	CLA	C3C-C4C-NC	2.40	113.40	110.43
14	B1	832	CLA	C3C-C4C-NC	2.40	113.40	110.43
14	B5	1812	CLA	C3B-C4B-NB	2.40	112.31	109.21
14	B2	836	CLA	C2C-C1C-NC	2.40	112.58	110.09
16	B4	850	BCR	C33-C5-C6	2.40	127.19	124.51
16	J4	103	BCR	C37-C22-C23	2.40	121.92	118.10
16	J1	103	BCR	C37-C22-C23	2.40	121.92	118.10
14	A4	841	CLA	C4-C3-C5	2.40	119.43	115.29
14	B6	804	CLA	O2D-CGD-CBD	2.40	115.54	111.28
16	M4	101	BCR	C38-C26-C25	2.40	127.20	124.51
14	J4	101	CLA	C4A-NA-C1A	2.40	109.42	106.32
14	B1	819	CLA	CED-O2D-CGD	2.40	121.51	115.97
14	A2	1643	CLA	CED-O2D-CGD	2.40	121.51	115.97
14	A2	1623	CLA	O2A-CGA-CBA	2.40	118.87	111.92
16	L2	208	BCR	C37-C22-C23	2.40	121.93	118.10
14	B6	814	CLA	C3C-C4C-NC	2.40	113.41	110.43
16	J4	104	BCR	C36-C18-C19	2.40	121.93	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A1	812	CLA	CED-O2D-CGD	2.40	121.51	115.97
14	B1	818	CLA	CED-O2D-CGD	2.40	121.51	115.97
14	A6	1611	CLA	CED-O2D-CGD	2.40	121.51	115.97
16	B5	1850	BCR	C36-C18-C19	2.40	121.93	118.10
14	B3	1824	CLA	CMB-C2B-C3B	2.40	129.26	124.88
14	A2	1618	CLA	CED-O2D-CGD	2.41	121.51	115.97
14	A6	1623	CLA	C3C-C4C-NC	2.41	113.41	110.43
14	J1	101	CLA	C2C-C1C-NC	2.41	112.58	110.09
14	A2	1629	CLA	C3C-C4C-NC	2.41	113.41	110.43
16	L6	209	BCR	C37-C22-C23	2.41	121.94	118.10
16	M1	1202	BCR	C32-C1-C6	2.41	114.21	110.31
16	J4	103	BCR	C32-C1-C6	2.41	114.21	110.31
14	A3	832	CLA	CED-O2D-CGD	2.41	121.52	115.97
16	A2	1652	BCR	C1-C6-C7	2.41	122.50	115.73
14	A1	810	CLA	CED-O2D-CGD	2.41	121.52	115.97
16	I1	103	BCR	C38-C26-C25	2.41	127.21	124.51
14	J4	101	CLA	CED-O2D-CGD	2.41	121.52	115.97
14	A6	1621	CLA	O2A-CGA-CBA	2.41	118.89	111.92
16	F4	201	BCR	C36-C18-C19	2.41	121.94	118.10
16	I4	102	BCR	C32-C1-C6	2.41	114.22	110.31
14	B1	825	CLA	C3C-C4C-NC	2.41	113.41	110.43
14	A2	1601	CLA	C3C-C4C-NC	2.41	113.41	110.43
14	A4	801	CLA	CGD-CBD-CAD	2.41	118.55	110.73
14	B5	1840	CLA	C2C-C1C-NC	2.41	112.59	110.09
14	B4	834	CLA	C3C-C4C-NC	2.41	113.42	110.43
14	A1	805	CLA	CED-O2D-CGD	2.41	121.53	115.97
14	A2	1615	CLA	C3C-C4C-NC	2.41	113.42	110.43
16	B4	847	BCR	C38-C26-C25	2.41	127.21	124.51
14	A5	827	CLA	C2C-C1C-NC	2.41	112.59	110.09
14	B3	1842	CLA	CAC-C3C-C4C	2.41	128.15	124.82
14	B1	825	CLA	C2C-C1C-NC	2.41	112.59	110.09
14	A4	823	CLA	CAC-C3C-C4C	2.42	128.15	124.82
14	A2	1642	CLA	CAC-C3C-C4C	2.42	128.15	124.82
14	A2	1620	CLA	C2C-C1C-NC	2.42	112.59	110.09
16	B3	1848	BCR	C38-C26-C25	2.42	127.21	124.51
14	B2	831	CLA	C3C-C4C-NC	2.42	113.42	110.43
14	L6	203	CLA	CMC-C2C-C1C	2.42	128.75	125.05
14	L3	202	CLA	C4A-NA-C1A	2.42	109.44	106.32
14	A3	813	CLA	CMB-C2B-C3B	2.42	129.28	124.88
14	A5	821	CLA	C3C-C4C-NC	2.42	113.42	110.43
16	A4	849	BCR	C1-C6-C7	2.42	122.53	115.73
16	M2	1202	BCR	C38-C26-C25	2.42	127.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B2	809	CLA	C3C-C4C-NC	2.42	113.42	110.43
14	B1	839	CLA	C2C-C1C-NC	2.42	112.59	110.09
14	B6	803	CLA	C2C-C1C-NC	2.42	112.60	110.09
14	B2	814	CLA	CMC-C2C-C1C	2.42	128.76	125.05
16	B1	849	BCR	C37-C22-C23	2.42	121.96	118.10
14	B3	1805	CLA	CED-O2D-CGD	2.42	121.55	115.97
14	A5	824	CLA	C3C-C4C-NC	2.42	113.43	110.43
14	A5	840	CLA	CAC-C3C-C4C	2.42	128.16	124.82
14	B4	829	CLA	CMC-C2C-C1C	2.42	128.76	125.05
14	A1	804	CLA	CED-O2D-CGD	2.42	121.55	115.97
14	A4	823	CLA	C3C-C4C-NC	2.42	113.43	110.43
16	I3	101	BCR	C38-C26-C25	2.42	127.22	124.51
14	A5	805	CLA	CMB-C2B-C3B	2.42	129.29	124.88
14	A2	1608	CLA	O2D-CGD-CBD	2.42	115.58	111.28
14	A4	820	CLA	O2A-CGA-CBA	2.43	118.93	111.92
14	J5	101	CLA	CED-O2D-CGD	2.43	121.56	115.97
14	X1	1701	CLA	C3C-C4C-NC	2.43	113.43	110.43
14	B4	801	CLA	O2A-CGA-CBA	2.43	118.94	111.92
14	A3	823	CLA	C3C-C4C-NC	2.43	113.44	110.43
14	A1	816	CLA	CED-O2D-CGD	2.43	121.57	115.97
14	A3	813	CLA	CAC-C3C-C4C	2.43	128.17	124.82
14	I1	101	CLA	O2A-CGA-CBA	2.43	118.94	111.92
14	A1	832	CLA	CED-O2D-CGD	2.43	121.57	115.97
16	A3	852	BCR	C33-C5-C6	2.43	127.23	124.51
14	B1	837	CLA	C3C-C4C-NC	2.43	113.44	110.43
16	L5	207	BCR	C38-C26-C25	2.43	127.23	124.51
14	A3	805	CLA	CHB-C4A-NA	2.43	127.87	124.51
16	I1	103	BCR	C37-C22-C23	2.43	121.97	118.10
16	J1	104	BCR	C32-C1-C6	2.43	114.25	110.31
14	B6	803	CLA	C3C-C4C-NC	2.43	113.44	110.43
14	B3	1822	CLA	C2C-C1C-NC	2.43	112.61	110.09
14	A1	822	CLA	C3C-C4C-NC	2.43	113.44	110.43
14	A1	831	CLA	C3C-C4C-NC	2.43	113.44	110.43
14	A3	811	CLA	CED-O2D-CGD	2.43	121.58	115.97
14	A4	814	CLA	C4A-NA-C1A	2.43	109.46	106.32
14	B3	1840	CLA	C2C-C1C-NC	2.44	112.61	110.09
14	A3	842	CLA	C2C-C1C-NC	2.44	112.61	110.09
14	X3	102	CLA	C3C-C4C-NC	2.44	113.44	110.43
14	A1	829	CLA	O2A-CGA-CBA	2.44	118.96	111.92
14	B5	1833	CLA	C3C-C4C-NC	2.44	113.44	110.43
14	B4	842	CLA	CAC-C3C-C4C	2.44	128.18	124.82
14	A5	832	CLA	CMB-C2B-C3B	2.44	129.32	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A4	818	CLA	CED-O2D-CGD	2.44	121.59	115.97
16	J6	1104	BCR	C32-C1-C6	2.44	114.26	110.31
16	F4	203	BCR	C33-C5-C6	2.44	127.24	124.51
14	A1	812	CLA	CAC-C3C-C4C	2.44	128.18	124.82
16	A4	846	BCR	C40-C30-C25	2.44	114.26	110.31
14	A6	1601	CLA	C4A-NA-C1A	2.44	109.47	106.32
16	A3	852	BCR	C1-C6-C7	2.44	122.59	115.73
14	A3	842	CLA	C1-O2A-CGA	2.44	122.39	116.77
14	A6	1621	CLA	C3C-C4C-NC	2.44	113.45	110.43
16	B3	1849	BCR	C36-C18-C19	2.44	121.99	118.10
16	B5	1850	BCR	C38-C26-C25	2.44	127.24	124.51
16	A5	853	BCR	C34-C9-C8	2.44	121.99	118.10
14	A5	827	CLA	C3C-C4C-NC	2.44	113.45	110.43
14	B6	821	CLA	C4A-NA-C1A	2.44	109.47	106.32
14	A5	828	CLA	C3B-C4B-NB	2.44	112.37	109.21
14	A6	1624	CLA	C3C-C4C-NC	2.44	113.45	110.43
16	B6	850	BCR	C38-C26-C25	2.44	127.24	124.51
14	B3	1820	CLA	C3B-C4B-NB	2.44	112.37	109.21
14	A4	826	CLA	C3C-C4C-NC	2.44	113.45	110.43
16	J3	103	BCR	C32-C1-C6	2.44	114.27	110.31
14	B1	854	CLA	C3B-C4B-NB	2.45	112.37	109.21
14	A4	853	CLA	C3C-C4C-NC	2.45	113.46	110.43
14	B4	825	CLA	C3C-C4C-NC	2.45	113.46	110.43
14	A1	812	CLA	C3C-C4C-NC	2.45	113.46	110.43
14	B1	806	CLA	CED-O2D-CGD	2.45	121.61	115.97
16	B3	1845	BCR	C37-C22-C23	2.45	122.00	118.10
14	A2	1644	CLA	C4-C3-C5	2.45	119.51	115.29
14	A4	829	CLA	C2C-C1C-NC	2.45	112.62	110.09
14	A2	1638	CLA	CMB-C2B-C3B	2.45	129.34	124.88
14	B5	1838	CLA	C3C-C4C-NC	2.45	113.46	110.43
14	B6	832	CLA	C3C-C4C-NC	2.45	113.46	110.43
14	B2	815	CLA	C3C-C4C-NC	2.45	113.46	110.43
16	A1	847	BCR	C1-C6-C7	2.45	122.61	115.73
16	L5	207	BCR	C37-C22-C23	2.45	122.00	118.10
14	A2	1636	CLA	CED-O2D-CGD	2.45	121.61	115.97
16	M5	101	BCR	C37-C22-C23	2.45	122.00	118.10
14	A2	1601	CLA	C4A-NA-C1A	2.45	109.48	106.32
14	B3	1819	CLA	C3C-C4C-NC	2.45	113.46	110.43
14	B3	1834	CLA	C3C-C4C-NC	2.45	113.46	110.43
14	B5	1812	CLA	C3C-C4C-NC	2.45	113.46	110.43
14	B4	801	CLA	CMC-C2C-C1C	2.45	128.81	125.05
14	B3	1806	CLA	C3C-C4C-NC	2.45	113.46	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1836	CLA	C2C-C1C-NC	2.45	112.63	110.09
16	A6	1652	BCR	C33-C5-C6	2.45	127.25	124.51
14	A2	1605	CLA	CAC-C3C-C4C	2.45	128.20	124.82
14	B6	840	CLA	CAC-C3C-C4C	2.45	128.20	124.82
14	B4	818	CLA	C3C-C4C-NC	2.45	113.47	110.43
14	I6	101	CLA	CED-O2D-CGD	2.45	121.62	115.97
14	L5	202	CLA	C4A-NA-C1A	2.45	109.49	106.32
16	A4	849	BCR	C33-C5-C6	2.45	127.25	124.51
14	B6	840	CLA	O2A-CGA-CBA	2.45	119.02	111.92
14	A4	840	CLA	C2C-C1C-NC	2.45	112.63	110.09
16	A4	847	BCR	C30-C25-C24	2.45	122.63	115.73
14	B1	823	CLA	CED-O2D-CGD	2.45	121.63	115.97
14	B2	818	CLA	CED-O2D-CGD	2.45	121.63	115.97
14	B3	1807	CLA	C3C-C4C-NC	2.46	113.47	110.43
14	A5	805	CLA	CHB-C4A-NA	2.46	127.91	124.51
14	B2	811	CLA	C4A-NA-C1A	2.46	109.49	106.32
16	B6	850	BCR	C8-C7-C6	2.46	134.13	127.25
14	B3	1812	CLA	C3B-C4B-NB	2.46	112.39	109.21
14	B6	838	CLA	CED-O2D-CGD	2.46	121.63	115.97
14	A5	833	CLA	C3C-C4C-NC	2.46	113.47	110.43
14	B5	1804	CLA	CMC-C2C-C1C	2.46	128.82	125.05
14	B5	1833	CLA	C2C-C1C-NC	2.46	112.64	110.09
16	J2	103	BCR	C32-C1-C6	2.46	114.30	110.31
14	A5	805	CLA	CED-O2D-CGD	2.46	121.64	115.97
14	B4	814	CLA	CED-O2D-CGD	2.46	121.64	115.97
16	L1	203	BCR	C36-C18-C19	2.46	122.02	118.10
14	M3	1601	CLA	CED-O2D-CGD	2.46	121.64	115.97
14	A5	803	CLA	CAC-C3C-C4C	2.46	128.21	124.82
14	B2	839	CLA	CAC-C3C-C4C	2.46	128.21	124.82
14	A3	821	CLA	O2A-CGA-CBA	2.46	119.03	111.92
14	A2	1613	CLA	C3C-C4C-NC	2.46	113.48	110.43
14	B5	1842	CLA	O2D-CGD-CBD	2.46	115.65	111.28
14	A3	801	CLA	CMC-C2C-C1C	2.46	128.82	125.05
14	B1	838	CLA	C2C-C1C-NC	2.46	112.64	110.09
14	A6	1605	CLA	CHB-C4A-NA	2.46	127.92	124.51
16	A5	853	BCR	C37-C22-C23	2.46	122.02	118.10
14	B1	835	CLA	C2C-C1C-NC	2.46	112.64	110.09
14	A5	835	CLA	CED-O2D-CGD	2.46	121.65	115.97
14	L6	203	CLA	CAC-C3C-C4C	2.46	128.22	124.82
14	A5	802	CLA	O2A-CGA-CBA	2.46	119.04	111.92
14	B6	810	CLA	C3C-C4C-NC	2.46	113.48	110.43
14	A4	822	CLA	C3C-C4C-NC	2.46	113.48	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B3	1826	CLA	C2C-C1C-NC	2.46	112.64	110.09
14	L1	201	CLA	CMB-C2B-C3B	2.47	129.37	124.88
14	A2	1625	CLA	C3C-C4C-NC	2.47	113.48	110.43
14	A1	838	CLA	C1-O2A-CGA	2.47	122.45	116.77
14	A4	838	CLA	C2C-C1C-NC	2.47	112.64	110.09
14	B5	1821	CLA	CED-O2D-CGD	2.47	121.65	115.97
14	A6	1602	CLA	CMC-C2C-C1C	2.47	128.83	125.05
14	B1	830	CLA	C3C-C4C-NC	2.47	113.48	110.43
14	A5	838	CLA	C3C-C4C-NC	2.47	113.48	110.43
14	B1	806	CLA	C2C-C1C-NC	2.47	112.64	110.09
14	A6	1618	CLA	CED-O2D-CGD	2.47	121.66	115.97
14	A5	823	CLA	C3C-C4C-NC	2.47	113.48	110.43
14	B6	817	CLA	CED-O2D-CGD	2.47	121.66	115.97
14	A6	1624	CLA	CAC-C3C-C4C	2.47	128.22	124.82
14	B5	1813	CLA	C3C-C4C-NC	2.47	113.49	110.43
16	J6	1105	BCR	C32-C1-C6	2.47	114.31	110.31
16	J5	104	BCR	C36-C18-C19	2.47	122.03	118.10
14	B4	838	CLA	C3C-C4C-NC	2.47	113.49	110.43
14	B5	1839	CLA	O2A-CGA-CBA	2.47	119.06	111.92
14	A5	802	CLA	CED-O2D-CGD	2.47	121.67	115.97
14	A3	843	CLA	CMC-C2C-C1C	2.47	128.84	125.05
14	A6	1617	CLA	CED-O2D-CGD	2.47	121.67	115.97
14	B3	1819	CLA	CED-O2D-CGD	2.47	121.67	115.97
16	A2	1652	BCR	C37-C22-C23	2.48	122.04	118.10
14	A2	1623	CLA	O2D-CGD-CBD	2.48	115.67	111.28
14	A4	837	CLA	CED-O2D-CGD	2.48	121.67	115.97
14	A3	817	CLA	CED-O2D-CGD	2.48	121.67	115.97
14	B5	1813	CLA	CED-O2D-CGD	2.48	121.67	115.97
14	A4	804	CLA	CHB-C4A-NA	2.48	127.94	124.51
14	B5	1842	CLA	O2A-CGA-CBA	2.48	119.08	111.92
14	X6	1701	CLA	C3C-C4C-NC	2.48	113.50	110.43
16	F6	201	BCR	C36-C18-C19	2.48	122.05	118.10
14	B1	820	CLA	CED-O2D-CGD	2.48	121.68	115.97
14	A6	1606	CLA	CED-O2D-CGD	2.48	121.68	115.97
14	B3	1814	CLA	CED-O2D-CGD	2.48	121.68	115.97
14	A3	819	CLA	CED-O2D-CGD	2.48	121.68	115.97
14	B4	822	CLA	C2C-C1C-NC	2.48	112.66	110.09
14	B6	820	CLA	C2C-C1C-NC	2.48	112.66	110.09
14	A2	1606	CLA	CMB-C2B-C3B	2.48	129.40	124.88
14	A3	810	CLA	C3C-C4C-NC	2.48	113.50	110.43
16	F3	201	BCR	C36-C18-C19	2.48	122.05	118.10
14	A5	821	CLA	O2A-CGA-CBA	2.48	119.10	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	805	CLA	CMC-C2C-C1C	2.48	128.85	125.05
16	A3	850	BCR	C30-C25-C24	2.48	122.71	115.73
16	B4	849	BCR	C29-C30-C25	2.48	114.36	110.48
16	B2	842	BCR	C37-C22-C23	2.48	122.05	118.10
16	A1	844	BCR	C37-C22-C23	2.48	122.05	118.10
16	A5	847	BCR	C37-C22-C23	2.48	122.05	118.10
14	A5	839	CLA	C3C-C4C-NC	2.48	113.50	110.43
14	A2	1607	CLA	CMB-C2B-C3B	2.48	129.40	124.88
14	A2	1644	CLA	CMC-C2C-C1C	2.48	128.86	125.05
16	F1	1302	BCR	C38-C26-C25	2.48	127.29	124.51
16	A3	849	BCR	C37-C22-C23	2.48	122.06	118.10
14	A5	830	CLA	C2C-C1C-NC	2.49	112.66	110.09
16	A1	845	BCR	C30-C25-C24	2.49	122.72	115.73
14	B4	833	CLA	C3C-C4C-NC	2.49	113.51	110.43
16	A6	1648	BCR	C1-C6-C7	2.49	122.72	115.73
14	A6	1634	CLA	CED-O2D-CGD	2.49	121.70	115.97
14	B6	818	CLA	C3B-C4B-NB	2.49	112.43	109.21
14	B6	822	CLA	CED-O2D-CGD	2.49	121.70	115.97
14	A5	818	CLA	C2C-C1C-NC	2.49	112.67	110.09
14	B6	802	CLA	O2A-CGA-CBA	2.49	119.12	111.92
14	B5	1824	CLA	CMB-C2B-C3B	2.49	129.41	124.88
16	B6	843	BCR	C37-C22-C23	2.49	122.06	118.10
14	B6	811	CLA	CED-O2D-CGD	2.49	121.71	115.97
14	B6	837	CLA	C2C-C1C-NC	2.49	112.67	110.09
14	B6	822	CLA	CMB-C2B-C3B	2.49	129.42	124.88
16	B1	843	BCR	C37-C22-C23	2.49	122.07	118.10
14	B5	1808	CLA	C4-C3-C5	2.49	119.59	115.29
14	B6	823	CLA	C3C-C4C-NC	2.49	113.52	110.43
14	A3	806	CLA	O2D-CGD-CBD	2.49	115.71	111.28
14	A5	834	CLA	CED-O2D-CGD	2.49	121.72	115.97
16	J2	102	BCR	C37-C22-C23	2.50	122.07	118.10
14	A4	840	CLA	C1-O2A-CGA	2.50	122.52	116.77
16	B1	847	BCR	C40-C30-C25	2.50	114.36	110.31
16	A5	848	BCR	C30-C25-C24	2.50	122.75	115.73
14	B4	833	CLA	C2C-C1C-NC	2.50	112.67	110.09
14	A3	806	CLA	CED-O2D-CGD	2.50	121.72	115.97
16	B1	849	BCR	C34-C9-C8	2.50	122.08	118.10
14	A4	829	CLA	O2A-CGA-CBA	2.50	119.14	111.92
14	L5	204	CLA	CMC-C2C-C1C	2.50	128.88	125.05
16	I5	101	BCR	C38-C26-C25	2.50	127.30	124.51
14	A1	820	CLA	C2C-C1C-NC	2.50	112.68	110.09
14	A4	824	CLA	C2C-C1C-NC	2.50	112.68	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B3	1830	CLA	C3C-C4C-NC	2.50	113.52	110.43
14	A6	1609	CLA	C3C-C4C-NC	2.50	113.52	110.43
14	B2	826	CLA	CMC-C2C-C1C	2.50	128.88	125.05
14	A5	841	CLA	C2C-C1C-NC	2.50	112.68	110.09
14	A2	1637	CLA	CED-O2D-CGD	2.50	121.73	115.97
16	B3	1847	BCR	C38-C26-C25	2.50	127.31	124.51
14	L6	202	CLA	C4A-NA-C1A	2.50	109.55	106.32
14	B5	1802	CLA	C3B-C4B-NB	2.50	112.44	109.21
14	B4	805	CLA	C2C-C1C-NC	2.50	112.68	110.09
16	A2	1650	BCR	C30-C25-C24	2.50	122.76	115.73
14	B3	1813	CLA	CED-O2D-CGD	2.50	121.73	115.97
14	A4	834	CLA	C3C-C4C-NC	2.50	113.53	110.43
14	A4	824	CLA	C3C-C4C-NC	2.50	113.53	110.43
14	A4	804	CLA	CMB-C2B-C3B	2.50	129.44	124.88
14	B1	814	CLA	CAC-C3C-C4C	2.50	128.27	124.82
14	A3	803	CLA	C2C-C1C-NC	2.50	112.68	110.09
14	L2	202	CLA	C3C-C4C-NC	2.50	113.53	110.43
14	B3	1833	CLA	C2C-C1C-NC	2.50	112.68	110.09
14	A4	802	CLA	CAC-C3C-C4C	2.50	128.27	124.82
14	A5	842	CLA	CAC-C3C-C4C	2.50	128.27	124.82
14	B4	807	CLA	C3C-C4C-NC	2.51	113.53	110.43
14	B3	1802	CLA	CED-O2D-CGD	2.51	121.74	115.97
14	B2	806	CLA	CED-O2D-CGD	2.51	121.74	115.97
14	A4	835	CLA	CMB-C2B-C3B	2.51	129.44	124.88
14	B6	807	CLA	C4-C3-C5	2.51	119.61	115.29
14	B5	1835	CLA	C2C-C1C-NC	2.51	112.69	110.09
14	B2	812	CLA	CAC-C3C-C4C	2.51	128.28	124.82
14	A2	1602	CLA	CMC-C2C-C1C	2.51	128.90	125.05
14	B4	819	CLA	CED-O2D-CGD	2.51	121.75	115.97
14	A1	834	CLA	CMB-C2B-C3B	2.51	129.45	124.88
14	F5	1301	CLA	C3C-C4C-NC	2.51	113.54	110.43
14	B3	1831	CLA	C3C-C4C-NC	2.51	113.54	110.43
16	B2	846	BCR	C36-C18-C19	2.51	122.10	118.10
14	A4	810	CLA	C3C-C4C-NC	2.51	113.54	110.43
14	A3	827	CLA	C3C-C4C-NC	2.51	113.54	110.43
14	L1	205	CLA	CMC-C2C-C1C	2.51	128.90	125.05
14	A3	802	CLA	O2A-CGA-CBA	2.51	119.19	111.92
14	A1	804	CLA	CMB-C2B-C3B	2.51	129.46	124.88
17	A3	854	LHG	C25-C24-C23	2.51	126.66	114.17
16	I1	102	BCR	C38-C26-C25	2.51	127.32	124.51
16	M5	101	BCR	C32-C1-C6	2.52	114.39	110.31
14	B4	804	CLA	CMC-C2C-C1C	2.52	128.91	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	807	CLA	CED-O2D-CGD	2.52	121.77	115.97
14	A4	803	CLA	C3C-C4C-NC	2.52	113.55	110.43
14	A3	809	CLA	C3C-C4C-NC	2.52	113.55	110.43
14	B5	1824	CLA	CED-O2D-CGD	2.52	121.77	115.97
14	A3	836	CLA	C3C-C4C-NC	2.52	113.55	110.43
14	A3	839	CLA	C3C-C4C-NC	2.52	113.55	110.43
16	J5	103	BCR	C37-C22-C23	2.52	122.11	118.10
14	A4	841	CLA	CMC-C2C-C1C	2.52	128.91	125.05
14	B2	801	CLA	O2D-CGD-CBD	2.52	115.75	111.28
14	I1	101	CLA	O2D-CGD-CBD	2.52	115.75	111.28
14	A2	1615	CLA	CAC-C3C-C4C	2.52	128.30	124.82
14	A1	824	CLA	C2C-C1C-NC	2.52	112.70	110.09
17	A6	1650	LHG	C25-C24-C23	2.52	126.70	114.17
16	A4	846	BCR	C38-C26-C25	2.52	127.33	124.51
14	B3	1825	CLA	C3C-C4C-NC	2.52	113.55	110.43
14	B6	811	CLA	C3C-C4C-NC	2.52	113.55	110.43
14	B3	1839	CLA	C2C-C1C-NC	2.52	112.70	110.09
14	A6	1605	CLA	CMB-C2B-C3B	2.52	129.48	124.88
14	A4	813	CLA	CED-O2D-CGD	2.52	121.79	115.97
16	B4	850	BCR	C37-C22-C23	2.52	122.12	118.10
16	B5	1849	BCR	C36-C18-C19	2.52	122.12	118.10
16	L2	203	BCR	C36-C18-C19	2.52	122.12	118.10
14	A3	843	CLA	C4-C3-C5	2.53	119.64	115.29
16	A5	850	BCR	C37-C22-C23	2.53	122.12	118.10
14	B6	810	CLA	C3B-C4B-NB	2.53	112.47	109.21
14	B1	803	CLA	C2C-C1C-NC	2.53	112.70	110.09
14	B2	817	CLA	C3B-C4B-NB	2.53	112.48	109.21
14	A4	831	CLA	CMB-C2B-C3B	2.53	129.48	124.88
16	A6	1648	BCR	C33-C5-C6	2.53	127.34	124.51
14	J6	1101	CLA	CAC-C3C-C4C	2.53	128.30	124.82
14	A4	814	CLA	CMB-C2B-C3B	2.53	129.48	124.88
14	B5	1814	CLA	C4A-NA-C1A	2.53	109.58	106.32
14	A5	825	CLA	C3C-C4C-NC	2.53	113.56	110.43
14	A6	1625	CLA	C3C-C4C-NC	2.53	113.56	110.43
16	B5	1845	BCR	C37-C22-C23	2.53	122.12	118.10
14	A2	1607	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	B6	824	CLA	C2C-C1C-NC	2.53	112.71	110.09
14	B1	801	CLA	O2A-CGA-CBA	2.53	119.23	111.92
14	A6	1638	CLA	C3C-C4C-NC	2.53	113.56	110.43
16	I3	102	BCR	C36-C18-C19	2.53	122.13	118.10
14	B3	1808	CLA	C4-C3-C5	2.53	119.65	115.29
14	J4	101	CLA	C3C-C4C-NC	2.53	113.56	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	802	CLA	C3B-C4B-NB	2.53	112.48	109.21
14	A6	1635	CLA	C3C-C4C-NC	2.53	113.56	110.43
14	B3	1803	CLA	O2D-CGD-CBD	2.53	115.77	111.28
16	I4	101	BCR	C29-C30-C25	2.53	114.44	110.48
14	B6	806	CLA	CMB-C2B-C3B	2.53	129.49	124.88
14	A3	815	CLA	CMB-C2B-C3B	2.53	129.49	124.88
14	B6	806	CLA	C3C-C4C-NC	2.53	113.56	110.43
16	J6	1104	BCR	C33-C5-C6	2.53	127.34	124.51
14	B4	839	CLA	C3C-C4C-NC	2.53	113.56	110.43
14	B1	808	CLA	O2D-CGD-CBD	2.53	115.78	111.28
14	A4	803	CLA	CMB-C2B-C3B	2.53	129.49	124.88
14	A2	1634	CLA	CMB-C2B-C3B	2.54	129.50	124.88
16	J1	104	BCR	C36-C18-C19	2.54	122.14	118.10
14	B1	802	CLA	CMB-C2B-C3B	2.54	129.50	124.88
14	B1	812	CLA	C3C-C4C-NC	2.54	113.57	110.43
14	A3	805	CLA	CMB-C2B-C3B	2.54	129.50	124.88
14	A2	1632	CLA	O2A-CGA-CBA	2.54	119.25	111.92
14	A3	803	CLA	CAC-C3C-C4C	2.54	128.32	124.82
14	B6	828	CLA	C3C-C4C-NC	2.54	113.57	110.43
14	B4	813	CLA	C3C-C4C-NC	2.54	113.57	110.43
14	B6	840	CLA	O2D-CGD-CBD	2.54	115.78	111.28
14	A5	803	CLA	C2C-C1C-NC	2.54	112.72	110.09
14	B3	1807	CLA	CMB-C2B-C3B	2.54	129.50	124.88
14	A5	808	CLA	CMC-C2C-C1C	2.54	128.94	125.05
14	A4	806	CLA	CED-O2D-CGD	2.54	121.82	115.97
14	B3	1812	CLA	C3C-C4C-NC	2.54	113.57	110.43
14	A6	1630	CLA	O2A-CGA-CBA	2.54	119.26	111.92
14	A5	836	CLA	CMB-C2B-C3B	2.54	129.51	124.88
16	I5	101	BCR	C29-C30-C25	2.54	114.45	110.48
14	B5	1823	CLA	CED-O2D-CGD	2.54	121.83	115.97
14	A1	806	CLA	CED-O2D-CGD	2.54	121.83	115.97
14	B5	1820	CLA	C3B-C4B-NB	2.54	112.50	109.21
14	B2	801	CLA	C3C-C4C-NC	2.54	113.58	110.43
14	A1	836	CLA	C3C-C4C-NC	2.54	113.58	110.43
19	B3	1850	LMG	O8-C28-C29	2.54	119.27	111.92
19	B6	848	LMG	O8-C28-C29	2.54	119.27	111.92
14	A3	830	CLA	C2C-C1C-NC	2.54	112.72	110.09
14	A3	825	CLA	C3C-C4C-NC	2.54	113.58	110.43
14	A6	1606	CLA	O2D-CGD-CBD	2.55	115.80	111.28
14	X3	102	CLA	C2C-C1C-NC	2.55	112.73	110.09
16	B4	849	BCR	C36-C18-C19	2.55	122.16	118.10
14	B4	824	CLA	CMB-C2B-C3B	2.55	129.52	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	K6	1401	CLA	C3C-C4C-NC	2.55	113.58	110.43
14	B1	831	CLA	C2C-C1C-NC	2.55	112.73	110.09
14	B4	839	CLA	O2A-CGA-CBA	2.55	119.29	111.92
14	B6	835	CLA	CED-O2D-CGD	2.55	121.84	115.97
16	M3	1602	BCR	C38-C26-C25	2.55	127.36	124.51
14	A1	814	CLA	CMB-C2B-C3B	2.55	129.52	124.88
14	M3	1601	CLA	C4A-NA-C1A	2.55	109.61	106.32
14	A6	1611	CLA	C3C-C4C-NC	2.55	113.58	110.43
14	L3	203	CLA	C3C-C4C-NC	2.55	113.58	110.43
14	F3	202	CLA	CED-O2D-CGD	2.55	121.85	115.97
14	B2	821	CLA	CMB-C2B-C3B	2.55	129.52	124.88
16	F5	1302	BCR	C33-C5-C6	2.55	127.36	124.51
14	A3	818	CLA	C3C-C4C-NC	2.55	113.59	110.43
14	A5	835	CLA	C3C-C4C-NC	2.55	113.59	110.43
14	B5	1840	CLA	CED-O2D-CGD	2.55	121.85	115.97
16	M1	1202	BCR	C38-C26-C25	2.55	127.36	124.51
14	L5	205	CLA	C2C-C1C-NC	2.55	112.73	110.09
14	A6	1603	CLA	CED-O2D-CGD	2.55	121.85	115.97
14	B4	843	CLA	C3C-C4C-NC	2.55	113.59	110.43
16	F2	203	BCR	C33-C5-C6	2.55	127.37	124.51
16	M5	101	BCR	C38-C26-C25	2.55	127.37	124.51
14	L6	203	CLA	C4-C3-C5	2.55	119.69	115.29
14	B1	838	CLA	C3C-C4C-NC	2.55	113.59	110.43
14	A5	839	CLA	C2C-C1C-NC	2.55	112.73	110.09
14	L5	202	CLA	CED-O2D-CGD	2.56	121.86	115.97
14	K4	1401	CLA	C3C-C4C-NC	2.56	113.59	110.43
16	I3	101	BCR	C29-C30-C25	2.56	114.47	110.48
14	A6	1607	CLA	CED-O2D-CGD	2.56	121.86	115.97
14	A2	1641	CLA	O2D-CGD-CBD	2.56	115.82	111.28
14	B1	807	CLA	CMB-C2B-C3B	2.56	129.54	124.88
14	B2	839	CLA	O2A-CGA-CBA	2.56	119.31	111.92
16	J3	103	BCR	C37-C22-C23	2.56	122.17	118.10
14	B2	805	CLA	C4-C3-C5	2.56	119.70	115.29
16	B3	1851	BCR	C38-C26-C25	2.56	127.37	124.51
14	B5	1807	CLA	C3C-C4C-NC	2.56	113.60	110.43
14	B2	833	CLA	C2C-C1C-NC	2.56	112.74	110.09
14	B1	823	CLA	CMB-C2B-C3B	2.56	129.54	124.88
14	B6	816	CLA	C3C-C4C-NC	2.56	113.60	110.43
16	F6	203	BCR	C33-C5-C6	2.56	127.37	124.51
14	B5	1807	CLA	CMB-C2B-C3B	2.56	129.54	124.88
16	I6	102	BCR	C38-C26-C25	2.56	127.38	124.51
16	M1	1202	BCR	C37-C22-C23	2.56	122.18	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1806	CLA	C3C-C4C-NC	2.56	113.60	110.43
14	L6	202	CLA	CMB-C2B-C3B	2.56	129.55	124.88
14	A1	807	CLA	CMC-C2C-C1C	2.57	128.98	125.05
16	L6	204	BCR	C36-C18-C19	2.57	122.19	118.10
14	A1	803	CLA	C3C-C4C-NC	2.57	113.61	110.43
16	B5	1848	BCR	C40-C30-C25	2.57	114.47	110.31
14	A5	832	CLA	CED-O2D-CGD	2.57	121.88	115.97
14	A3	804	CLA	C3C-C4C-NC	2.57	113.61	110.43
14	B5	1808	CLA	O2A-CGA-CBA	2.57	119.34	111.92
14	A2	1619	CLA	CED-O2D-CGD	2.57	121.89	115.97
16	F6	203	BCR	C38-C26-C25	2.57	127.38	124.51
14	A3	832	CLA	C3C-C4C-NC	2.57	113.61	110.43
14	B6	840	CLA	C3C-C4C-NC	2.57	113.61	110.43
14	A1	804	CLA	CHB-C4A-NA	2.57	128.06	124.51
14	B1	839	CLA	CED-O2D-CGD	2.57	121.89	115.97
14	B4	836	CLA	C2C-C1C-NC	2.57	112.75	110.09
14	A2	1609	CLA	CED-O2D-CGD	2.57	121.89	115.97
16	A3	849	BCR	C1-C6-C7	2.57	122.95	115.73
14	B2	810	CLA	CED-O2D-CGD	2.57	121.89	115.97
14	B2	839	CLA	O2D-CGD-CBD	2.57	115.84	111.28
14	A5	809	CLA	C3C-C4C-NC	2.57	113.61	110.43
16	F2	203	BCR	C38-C26-C25	2.57	127.39	124.51
14	B1	812	CLA	CED-O2D-CGD	2.57	121.89	115.97
14	B5	1816	CLA	C3C-C4C-NC	2.57	113.61	110.43
14	B1	804	CLA	C3C-C4C-NC	2.57	113.61	110.43
14	B5	1839	CLA	C2C-C1C-NC	2.57	112.75	110.09
14	L4	203	CLA	C3C-C4C-NC	2.57	113.61	110.43
14	B5	1830	CLA	C3C-C4C-NC	2.57	113.61	110.43
14	I1	101	CLA	CAC-C3C-C4C	2.57	128.37	124.82
14	M3	1601	CLA	C3C-C4C-NC	2.57	113.61	110.43
14	A2	1615	CLA	CED-O2D-CGD	2.57	121.90	115.97
14	A1	802	CLA	CAC-C3C-C4C	2.57	128.37	124.82
14	A2	1604	CLA	C3B-C4B-NB	2.57	112.54	109.21
14	B4	835	CLA	C2C-C1C-NC	2.58	112.76	110.09
16	F4	203	BCR	C38-C26-C25	2.58	127.39	124.51
16	A4	846	BCR	C1-C6-C7	2.58	122.97	115.73
14	B2	836	CLA	C3C-C4C-NC	2.58	113.62	110.43
14	B6	834	CLA	C2C-C1C-NC	2.58	112.76	110.09
14	A1	802	CLA	C2C-C1C-NC	2.58	112.76	110.09
14	X2	1701	CLA	C2C-C1C-NC	2.58	112.76	110.09
14	A1	838	CLA	C2C-C1C-NC	2.58	112.76	110.09
14	A2	1605	CLA	C2C-C1C-NC	2.58	112.76	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	813	CLA	CAC-C3C-C4C	2.58	128.38	124.82
14	M6	1201	CLA	C3C-C4C-NC	2.58	113.62	110.43
14	A2	1617	CLA	CMB-C2B-C3B	2.58	129.58	124.88
14	B5	1803	CLA	C3C-C4C-NC	2.58	113.62	110.43
14	B2	830	CLA	C2C-C1C-NC	2.58	112.76	110.09
14	J5	101	CLA	C2C-C1C-NC	2.58	112.76	110.09
14	A4	817	CLA	C2C-C1C-NC	2.58	112.76	110.09
14	B4	842	CLA	CED-O2D-CGD	2.58	121.92	115.97
16	A6	1647	BCR	C2-C1-C6	2.58	114.51	110.48
14	A6	1608	CLA	CMC-C2C-C1C	2.58	129.01	125.05
14	A1	820	CLA	O2D-CGD-CBD	2.58	115.86	111.28
16	B4	848	BCR	C40-C30-C25	2.58	114.50	110.31
14	A1	810	CLA	C3C-C4C-NC	2.58	113.63	110.43
14	B4	806	CLA	C3C-C4C-NC	2.58	113.63	110.43
14	K1	1401	CLA	C3C-C4C-NC	2.58	113.63	110.43
14	A5	825	CLA	C2C-C1C-NC	2.58	112.77	110.09
14	X6	1701	CLA	C2C-C1C-NC	2.58	112.77	110.09
14	B5	1822	CLA	C2C-C1C-NC	2.58	112.77	110.09
14	B4	842	CLA	O2A-CGA-CBA	2.58	119.39	111.92
16	F5	1302	BCR	C38-C26-C25	2.58	127.40	124.51
14	B3	1843	CLA	C3C-C4C-NC	2.58	113.63	110.43
14	A2	1621	CLA	CED-O2D-CGD	2.58	121.93	115.97
16	I4	101	BCR	C38-C26-C25	2.59	127.40	124.51
14	B6	837	CLA	C3C-C4C-NC	2.59	113.63	110.43
14	A1	824	CLA	C3C-C4C-NC	2.59	113.63	110.43
14	B2	807	CLA	C3C-C4C-NC	2.59	113.63	110.43
14	B3	1837	CLA	O2D-CGD-CBD	2.59	115.87	111.28
14	A3	825	CLA	C2C-C1C-NC	2.59	112.77	110.09
14	A4	809	CLA	C3C-C4C-NC	2.59	113.63	110.43
16	A5	850	BCR	C33-C5-C6	2.59	127.40	124.51
16	L3	206	BCR	C38-C26-C25	2.59	127.40	124.51
14	B5	1828	CLA	C2C-C1C-NC	2.59	112.77	110.09
14	A2	1620	CLA	C3C-C4C-NC	2.59	113.63	110.43
14	B1	808	CLA	C4-C3-C5	2.59	119.75	115.29
14	A1	801	CLA	OBD-CAD-C3D	2.59	132.80	128.09
16	J2	102	BCR	C32-C1-C6	2.59	114.50	110.31
14	A4	801	CLA	CMC-C2C-C1C	2.59	129.02	125.05
14	A3	837	CLA	CMB-C2B-C3B	2.59	129.59	124.88
14	A3	808	CLA	CMC-C2C-C1C	2.59	129.02	125.05
14	A6	1603	CLA	C3B-C4B-NB	2.59	112.56	109.21
14	A5	833	CLA	C3B-C4B-NB	2.59	112.56	109.21
14	A3	833	CLA	O2A-CGA-CBA	2.59	119.41	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A4	813	CLA	C2C-C1C-NC	2.59	112.77	110.09
16	B6	845	BCR	C38-C26-C25	2.59	127.41	124.51
14	L1	205	CLA	C3C-C4C-NC	2.59	113.64	110.43
14	B3	1836	CLA	C2C-C1C-NC	2.59	112.77	110.09
14	B3	1803	CLA	CED-O2D-CGD	2.59	121.94	115.97
16	M3	1602	BCR	C37-C22-C23	2.59	122.23	118.10
14	A5	801	CLA	CMC-C2C-C1C	2.59	129.02	125.05
14	B5	1802	CLA	CED-O2D-CGD	2.59	121.95	115.97
14	J2	101	CLA	C2C-C1C-NC	2.59	112.78	110.09
14	A3	821	CLA	O2D-CGD-CBD	2.59	115.88	111.28
14	B4	830	CLA	C3C-C4C-NC	2.59	113.64	110.43
16	F3	201	BCR	C34-C9-C8	2.59	122.23	118.10
14	A1	829	CLA	C2C-C1C-NC	2.59	112.78	110.09
14	B4	802	CLA	C3B-C4B-NB	2.60	112.56	109.21
14	B2	816	CLA	C2C-C1C-NC	2.60	112.78	110.09
14	B5	1802	CLA	CMB-C2B-C3B	2.60	129.61	124.88
14	B4	840	CLA	C2C-C1C-NC	2.60	112.78	110.09
14	A1	817	CLA	C2C-C1C-NC	2.60	112.78	110.09
14	A5	810	CLA	C3C-C4C-NC	2.60	113.64	110.43
14	A4	805	CLA	O2D-CGD-CBD	2.60	115.89	111.28
14	A5	841	CLA	C1-O2A-CGA	2.60	122.75	116.77
14	B6	820	CLA	C4A-NA-C1A	2.60	109.67	106.32
16	J4	104	BCR	C32-C1-C6	2.60	114.52	110.31
14	B1	854	CLA	C3C-C4C-NC	2.60	113.65	110.43
14	B5	1815	CLA	C3C-C4C-NC	2.60	113.65	110.43
14	A6	1615	CLA	CMB-C2B-C3B	2.60	129.61	124.88
14	B1	833	CLA	C2C-C1C-NC	2.60	112.78	110.09
14	A4	815	CLA	C3C-C4C-NC	2.60	113.65	110.43
14	B3	1808	CLA	O2A-CGA-CBA	2.60	119.44	111.92
16	A2	1649	BCR	C1-C6-C7	2.60	123.04	115.73
14	B4	808	CLA	C4-C3-C5	2.60	119.77	115.29
14	B2	804	CLA	C3B-C4B-NB	2.60	112.57	109.21
16	A6	1645	BCR	C38-C26-C25	2.60	127.42	124.51
14	B1	811	CLA	C3C-C4C-NC	2.60	113.65	110.43
14	L3	202	CLA	CED-O2D-CGD	2.60	121.97	115.97
14	A6	1636	CLA	CMB-C2B-C3B	2.60	129.62	124.88
16	J3	103	BCR	C33-C5-C6	2.60	127.42	124.51
14	B3	1818	CLA	C3C-C4C-NC	2.60	113.65	110.43
14	A4	820	CLA	O2D-CGD-CBD	2.60	115.90	111.28
14	B5	1831	CLA	C3B-C4B-NB	2.60	112.58	109.21
14	A1	839	CLA	CMC-C2C-C1C	2.60	129.04	125.05
14	A5	839	CLA	CED-O2D-CGD	2.60	121.97	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	K3	1401	CLA	C3C-C4C-NC	2.61	113.66	110.43
14	B4	803	CLA	O2D-CGD-CBD	2.61	115.90	111.28
14	B4	810	CLA	C3C-C4C-NC	2.61	113.66	110.43
14	B3	1838	CLA	C3C-C4C-NC	2.61	113.66	110.43
16	A5	847	BCR	C1-C6-C7	2.61	123.06	115.73
14	A2	1628	CLA	O2A-CGA-CBA	2.61	119.46	111.92
16	A3	851	BCR	C2-C1-C6	2.61	114.56	110.48
14	A2	1644	CLA	C3C-C4C-NC	2.61	113.66	110.43
14	K2	1401	CLA	C3C-C4C-NC	2.61	113.66	110.43
14	B1	834	CLA	C2C-C1C-NC	2.61	112.79	110.09
14	A5	842	CLA	CMC-C2C-C1C	2.61	129.05	125.05
16	A2	1647	BCR	C37-C22-C23	2.61	122.26	118.10
14	B5	1839	CLA	C3C-C4C-NC	2.61	113.66	110.43
14	A4	819	CLA	C4A-NA-C1A	2.61	109.69	106.32
14	L1	206	CLA	C2C-C1C-NC	2.61	112.80	110.09
14	B3	1842	CLA	O2D-CGD-CBD	2.61	115.92	111.28
14	A4	841	CLA	C3C-C4C-NC	2.61	113.66	110.43
19	B2	848	LMG	O8-C28-C29	2.61	119.47	111.92
14	B3	1826	CLA	CED-O2D-CGD	2.61	121.99	115.97
16	A1	844	BCR	C1-C6-C7	2.61	123.08	115.73
16	I1	103	BCR	C36-C18-C19	2.61	122.26	118.10
14	B3	1839	CLA	C3C-C4C-NC	2.61	113.67	110.43
14	A6	1621	CLA	C2C-C1C-NC	2.61	112.80	110.09
14	A4	820	CLA	C2C-C1C-NC	2.61	112.80	110.09
16	A3	849	BCR	C38-C26-C25	2.61	127.44	124.51
14	F4	202	CLA	C3C-C4C-NC	2.62	113.67	110.43
14	B2	812	CLA	C3C-C4C-NC	2.62	113.67	110.43
19	B1	850	LMG	O8-C28-C29	2.62	119.48	111.92
14	B4	852	CLA	C3C-C4C-NC	2.62	113.67	110.43
14	B3	1841	CLA	C3C-C4C-NC	2.62	113.67	110.43
16	J5	104	BCR	C32-C1-C6	2.62	114.55	110.31
14	A1	817	CLA	C3C-C4C-NC	2.62	113.67	110.43
16	I1	102	BCR	C29-C30-C25	2.62	114.57	110.48
14	B5	1818	CLA	C3C-C4C-NC	2.62	113.67	110.43
14	B4	837	CLA	O2D-CGD-CBD	2.62	115.93	111.28
14	X4	102	CLA	C2C-C1C-NC	2.62	112.80	110.09
14	B4	801	CLA	CED-O2D-CGD	2.62	122.01	115.97
14	A1	829	CLA	C3C-C4C-NC	2.62	113.67	110.43
14	A4	838	CLA	O2D-CGD-CBD	2.62	115.93	111.28
14	A3	840	CLA	O2D-CGD-CBD	2.62	115.93	111.28
16	A2	1651	BCR	C2-C1-C6	2.62	114.58	110.48
14	B2	805	CLA	O2A-CGA-CBA	2.62	119.50	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1832	CLA	C2C-C1C-NC	2.62	112.81	110.09
14	B3	1813	CLA	C3C-C4C-NC	2.62	113.67	110.43
14	B2	839	CLA	C3C-C4C-NC	2.62	113.67	110.43
14	A4	808	CLA	C3C-C4C-NC	2.62	113.68	110.43
14	A5	832	CLA	C3C-C4C-NC	2.62	113.68	110.43
14	A6	1618	CLA	C2C-C1C-NC	2.62	112.81	110.09
16	B4	845	BCR	C37-C22-C23	2.62	122.28	118.10
16	I2	101	BCR	C29-C30-C25	2.63	114.58	110.48
14	B5	1815	CLA	CMB-C2B-C3B	2.63	129.66	124.88
14	A1	808	CLA	C3C-C4C-NC	2.63	113.68	110.43
14	B4	841	CLA	C3C-C4C-NC	2.63	113.68	110.43
14	B4	802	CLA	CED-O2D-CGD	2.63	122.02	115.97
14	M2	1201	CLA	C3C-C4C-NC	2.63	113.68	110.43
14	B5	1801	CLA	C3C-C4C-NC	2.63	113.68	110.43
16	A2	1648	BCR	C32-C1-C6	2.63	114.57	110.31
14	L4	201	CLA	O2A-CGA-CBA	2.63	119.51	111.92
14	B6	841	CLA	C3C-C4C-NC	2.63	113.68	110.43
14	A1	831	CLA	O2A-CGA-CBA	2.63	119.52	111.92
14	A1	801	CLA	CMC-C2C-C1C	2.63	129.08	125.05
14	B1	836	CLA	C3C-C4C-NC	2.63	113.68	110.43
14	A2	1606	CLA	C3C-C4C-NC	2.63	113.68	110.43
14	A4	817	CLA	C3C-C4C-NC	2.63	113.68	110.43
14	B6	804	CLA	C3C-C4C-NC	2.63	113.68	110.43
14	A3	818	CLA	C2C-C1C-NC	2.63	112.81	110.09
14	A4	820	CLA	CED-O2D-CGD	2.63	122.03	115.97
14	B6	836	CLA	C3C-C4C-NC	2.63	113.69	110.43
16	A6	1645	BCR	C37-C22-C23	2.63	122.29	118.10
14	J6	1102	CLA	C2C-C1C-NC	2.63	112.81	110.09
14	A2	1632	CLA	C2C-C1C-NC	2.63	112.81	110.09
14	A3	821	CLA	C2C-C1C-NC	2.63	112.81	110.09
14	L6	202	CLA	C3C-C4C-NC	2.63	113.69	110.43
14	B2	804	CLA	C3C-C4C-NC	2.63	113.69	110.43
14	K5	102	CLA	C3C-C4C-NC	2.63	113.69	110.43
14	B5	1819	CLA	CED-O2D-CGD	2.63	122.04	115.97
14	A4	825	CLA	O2A-CGA-CBA	2.63	119.53	111.92
14	B4	813	CLA	CED-O2D-CGD	2.63	122.04	115.97
14	B5	1815	CLA	CAC-C3C-C4C	2.63	128.45	124.82
14	B2	804	CLA	CMB-C2B-C3B	2.63	129.68	124.88
14	X1	1701	CLA	C2C-C1C-NC	2.63	112.82	110.09
14	B6	803	CLA	O2D-CGD-CBD	2.64	115.95	111.28
16	A6	1652	BCR	C29-C30-C25	2.64	114.60	110.48
14	B1	815	CLA	C3C-C4C-NC	2.64	113.69	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A2	1602	CLA	CGD-CBD-CAD	2.64	119.27	110.73
14	B2	829	CLA	C2C-C1C-NC	2.64	112.82	110.09
16	A5	849	BCR	C2-C1-C6	2.64	114.60	110.48
14	A4	833	CLA	C2C-C1C-NC	2.64	112.82	110.09
14	F2	202	CLA	C3C-C4C-NC	2.64	113.69	110.43
14	B1	814	CLA	C3C-C4C-NC	2.64	113.69	110.43
14	B3	1814	CLA	C4A-NA-C1A	2.64	109.72	106.32
14	A1	815	CLA	C3C-C4C-NC	2.64	113.69	110.43
16	F3	203	BCR	C33-C5-C6	2.64	127.46	124.51
14	A6	1610	CLA	C3C-C4C-NC	2.64	113.69	110.43
14	A2	1610	CLA	CMC-C2C-C1C	2.64	129.09	125.05
16	M6	1202	BCR	C37-C22-C23	2.64	122.30	118.10
14	A6	1601	CLA	C3C-C4C-NC	2.64	113.70	110.43
14	A2	1634	CLA	C3C-C4C-NC	2.64	113.70	110.43
16	A4	845	BCR	C32-C1-C6	2.64	114.59	110.31
16	L5	207	BCR	C36-C18-C19	2.64	122.30	118.10
14	B4	831	CLA	C3C-C4C-NC	2.64	113.70	110.43
14	B6	829	CLA	C3C-C4C-NC	2.64	113.70	110.43
14	A5	801	CLA	C3C-C4C-NC	2.64	113.70	110.43
14	A2	1619	CLA	C3C-C4C-NC	2.64	113.70	110.43
14	A2	1602	CLA	C3C-C4C-NC	2.64	113.70	110.43
14	A5	806	CLA	CBA-CAA-C2A	2.64	121.65	113.82
14	A3	826	CLA	O2A-CGA-CBA	2.64	119.56	111.92
14	B3	1842	CLA	C3C-C4C-NC	2.64	113.70	110.43
14	A2	1627	CLA	C2C-C1C-NC	2.64	112.83	110.09
16	J6	1104	BCR	C37-C22-C23	2.64	122.31	118.10
14	A5	830	CLA	C3C-C4C-NC	2.64	113.70	110.43
14	A3	830	CLA	O2A-CGA-CBA	2.64	119.56	111.92
14	L6	208	CLA	O2A-CGA-CBA	2.64	119.56	111.92
14	A1	820	CLA	C11-C10-C8	2.64	124.42	115.73
14	B1	807	CLA	C3B-C4B-NB	2.64	112.63	109.21
19	B4	851	LMG	O8-C28-C29	2.64	119.57	111.92
16	A6	1645	BCR	C1-C6-C7	2.64	123.16	115.73
14	A4	805	CLA	CBA-CAA-C2A	2.64	121.66	113.82
14	B4	803	CLA	C3C-C4C-NC	2.65	113.70	110.43
14	A2	1618	CLA	C3C-C4C-NC	2.65	113.70	110.43
14	L3	203	CLA	C2C-C1C-NC	2.65	112.83	110.09
14	B5	1842	CLA	CAC-C3C-C4C	2.65	128.47	124.82
16	A3	852	BCR	C37-C22-C23	2.65	122.32	118.10
14	B4	842	CLA	O2D-CGD-CBD	2.65	115.98	111.28
14	J4	101	CLA	C2C-C1C-NC	2.65	112.83	110.09
14	B6	806	CLA	C3B-C4B-NB	2.65	112.63	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L4	206	BCR	C36-C18-C19	2.65	122.32	118.10
14	A3	832	CLA	CMB-C2B-C3B	2.65	129.71	124.88
16	F1	1302	BCR	C33-C5-C6	2.65	127.47	124.51
14	A2	1611	CLA	C3C-C4C-NC	2.65	113.71	110.43
14	B5	1841	CLA	C3C-C4C-NC	2.65	113.71	110.43
14	A6	1630	CLA	C2C-C1C-NC	2.65	112.83	110.09
14	A5	811	CLA	C3C-C4C-NC	2.65	113.71	110.43
14	I1	101	CLA	C3C-C4C-NC	2.65	113.71	110.43
16	F6	201	BCR	C34-C9-C8	2.65	122.32	118.10
14	B1	827	CLA	C2C-C1C-NC	2.65	112.84	110.09
14	A2	1627	CLA	C3C-C4C-NC	2.65	113.71	110.43
14	B5	1810	CLA	C3C-C4C-NC	2.65	113.71	110.43
14	A4	832	CLA	O2A-CGA-CBA	2.65	119.59	111.92
14	B4	828	CLA	C2C-C1C-NC	2.66	112.84	110.09
14	B1	817	CLA	C3C-C4C-NC	2.66	113.72	110.43
14	A6	1633	CLA	C3C-C4C-NC	2.66	113.72	110.43
14	B1	812	CLA	C2C-C1C-NC	2.66	112.84	110.09
14	J6	1101	CLA	C2C-C1C-NC	2.66	112.84	110.09
14	M1	1201	CLA	C3C-C4C-NC	2.66	113.72	110.43
14	A2	1623	CLA	CED-O2D-CGD	2.66	122.10	115.97
14	B4	842	CLA	C3C-C4C-NC	2.66	113.72	110.43
14	L1	201	CLA	CED-O2D-CGD	2.66	122.10	115.97
16	B2	850	BCR	C38-C26-C25	2.66	127.48	124.51
14	B2	827	CLA	C3C-C4C-NC	2.66	113.72	110.43
14	L4	201	CLA	C3C-C4C-NC	2.66	113.72	110.43
14	A4	807	CLA	CMC-C2C-C1C	2.66	129.13	125.05
14	L5	202	CLA	C3C-C4C-NC	2.66	113.72	110.43
14	B4	802	CLA	CMB-C2B-C3B	2.66	129.73	124.88
14	A1	825	CLA	O2A-CGA-CBA	2.66	119.62	111.92
14	L6	206	CLA	C3C-C4C-NC	2.66	113.72	110.43
14	L4	204	CLA	C2C-C1C-NC	2.66	112.85	110.09
14	A5	806	CLA	CED-O2D-CGD	2.66	122.11	115.97
14	A1	831	CLA	C3B-C4B-NB	2.66	112.65	109.21
14	A6	1604	CLA	C3C-C4C-NC	2.66	113.73	110.43
14	B2	835	CLA	C3C-C4C-NC	2.66	113.73	110.43
16	M4	101	BCR	C37-C22-C23	2.66	122.34	118.10
14	A5	832	CLA	C4A-NA-C1A	2.66	109.76	106.32
14	A6	1632	CLA	O2A-CGA-CBA	2.66	119.62	111.92
14	A6	1601	CLA	CED-O2D-CGD	2.66	122.11	115.97
14	A5	815	CLA	CMB-C2B-C3B	2.66	129.73	124.88
14	A3	843	CLA	C3C-C4C-NC	2.67	113.73	110.43
16	A5	846	BCR	C29-C30-C25	2.67	114.64	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L3	201	BCR	C38-C26-C25	2.67	127.49	124.51
14	J3	101	CLA	C2C-C1C-NC	2.67	112.85	110.09
14	B3	1801	CLA	C3C-C4C-NC	2.67	113.73	110.43
14	B2	828	CLA	C3C-C4C-NC	2.67	113.73	110.43
14	B6	807	CLA	O2A-CGA-CBA	2.67	119.63	111.92
16	J1	103	BCR	C32-C1-C6	2.67	114.63	110.31
16	A1	843	BCR	C29-C30-C25	2.67	114.65	110.48
14	B1	829	CLA	C3C-C4C-NC	2.67	113.73	110.43
14	B4	808	CLA	O2A-CGA-CBA	2.67	119.64	111.92
14	B2	832	CLA	C2C-C1C-NC	2.67	112.86	110.09
16	F2	201	BCR	C34-C9-C8	2.67	122.35	118.10
14	B3	1839	CLA	O2A-CGA-CBA	2.67	119.64	111.92
14	B3	1840	CLA	CED-O2D-CGD	2.67	122.13	115.97
16	A6	1648	BCR	C37-C22-C23	2.67	122.36	118.10
19	B5	1851	LMG	O8-C28-C29	2.67	119.65	111.92
16	B4	850	BCR	C29-C30-C25	2.67	114.66	110.48
14	A2	1635	CLA	C3B-C4B-NB	2.67	112.67	109.21
14	A6	1630	CLA	C3C-C4C-NC	2.67	113.74	110.43
16	A6	1644	BCR	C29-C30-C25	2.67	114.66	110.48
14	F6	202	CLA	C3C-C4C-NC	2.67	113.74	110.43
14	A5	818	CLA	C3C-C4C-NC	2.67	113.74	110.43
14	A4	831	CLA	C4A-NA-C1A	2.67	109.77	106.32
14	B1	816	CLA	C2C-C1C-NC	2.67	112.86	110.09
14	A2	1604	CLA	CMB-C2B-C3B	2.67	129.75	124.88
14	A6	1603	CLA	CMB-C2B-C3B	2.68	129.75	124.88
14	B3	1817	CLA	C2C-C1C-NC	2.68	112.86	110.09
14	B5	1805	CLA	CED-O2D-CGD	2.68	122.14	115.97
16	M6	1202	BCR	C38-C26-C25	2.68	127.50	124.51
14	A5	821	CLA	O2D-CGD-CBD	2.68	116.03	111.28
14	B3	1802	CLA	C3B-C4B-NB	2.68	112.67	109.21
16	A5	845	BCR	C37-C22-C23	2.68	122.36	118.10
14	L6	207	CLA	O2A-CGA-CBA	2.68	119.66	111.92
14	A2	1643	CLA	C1-O2A-CGA	2.68	122.94	116.77
14	B2	834	CLA	C3C-C4C-NC	2.68	113.75	110.43
14	B1	821	CLA	C2C-C1C-NC	2.68	112.86	110.09
14	L1	201	CLA	C3C-C4C-NC	2.68	113.75	110.43
16	A2	1648	BCR	C29-C30-C25	2.68	114.67	110.48
14	A4	838	CLA	CED-O2D-CGD	2.68	122.15	115.97
14	B3	1835	CLA	C2C-C1C-NC	2.68	112.87	110.09
14	A1	809	CLA	C3C-C4C-NC	2.68	113.75	110.43
16	L3	201	BCR	C29-C30-C25	2.68	114.67	110.48
16	L6	209	BCR	C36-C18-C19	2.68	122.37	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	830	CLA	C3C-C4C-NC	2.68	113.75	110.43
14	L3	202	CLA	C3C-C4C-NC	2.68	113.75	110.43
16	L2	208	BCR	C36-C18-C19	2.68	122.38	118.10
14	A6	1618	CLA	C3C-C4C-NC	2.69	113.75	110.43
14	B4	831	CLA	C3B-C4B-NB	2.69	112.68	109.21
16	B4	849	BCR	C40-C30-C25	2.69	114.67	110.31
16	F3	203	BCR	C38-C26-C25	2.69	127.52	124.51
14	B2	836	CLA	O2A-CGA-CBA	2.69	119.69	111.92
16	B3	1848	BCR	C40-C30-C25	2.69	114.67	110.31
14	A4	801	CLA	C3C-C4C-NC	2.69	113.76	110.43
14	B2	828	CLA	C3B-C4B-NB	2.69	112.69	109.21
14	A6	1628	CLA	CMB-C2B-C3B	2.69	129.78	124.88
14	B5	1829	CLA	CMC-C2C-C1C	2.69	129.17	125.05
16	A3	856	BCR	C29-C30-C25	2.69	114.68	110.48
14	B6	813	CLA	C3C-C4C-NC	2.69	113.76	110.43
14	B3	1842	CLA	CED-O2D-CGD	2.69	122.17	115.97
14	A1	805	CLA	CBA-CAA-C2A	2.69	121.80	113.82
14	A4	829	CLA	C3C-C4C-NC	2.69	113.76	110.43
14	L6	207	CLA	C2C-C1C-NC	2.69	112.88	110.09
14	A6	1625	CLA	C2C-C1C-NC	2.69	112.88	110.09
14	L3	204	CLA	C2C-C1C-NC	2.69	112.88	110.09
16	B3	1848	BCR	C29-C30-C25	2.69	114.69	110.48
14	A5	826	CLA	O2A-CGA-CBA	2.69	119.71	111.92
14	A1	801	CLA	C3C-C4C-NC	2.69	113.76	110.43
14	B4	807	CLA	CMB-C2B-C3B	2.69	129.79	124.88
14	A2	1623	CLA	C2C-C1C-NC	2.70	112.88	110.09
14	B2	831	CLA	C2C-C1C-NC	2.70	112.89	110.09
14	A4	833	CLA	CED-O2D-CGD	2.70	122.19	115.97
14	B2	803	CLA	CED-O2D-CGD	2.70	122.19	115.97
14	A3	820	CLA	C4A-NA-C1A	2.70	109.81	106.32
14	B2	819	CLA	C4A-NA-C1A	2.70	109.81	106.32
14	F3	202	CLA	C3C-C4C-NC	2.70	113.77	110.43
14	A2	1601	CLA	CED-O2D-CGD	2.70	122.20	115.97
16	L1	209	BCR	C38-C26-C25	2.70	127.53	124.51
14	A2	1612	CLA	C3C-C4C-NC	2.70	113.77	110.43
14	B2	838	CLA	C3C-C4C-NC	2.70	113.77	110.43
14	B5	1843	CLA	C3C-C4C-NC	2.70	113.78	110.43
16	A5	847	BCR	C38-C26-C25	2.71	127.54	124.51
14	J5	102	CLA	C2C-C1C-NC	2.71	112.89	110.09
14	B6	827	CLA	CMC-C2C-C1C	2.71	129.20	125.05
14	B1	828	CLA	CMC-C2C-C1C	2.71	129.20	125.05
16	A1	844	BCR	C38-C26-C25	2.71	127.54	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	834	CLA	C3C-C4C-NC	2.71	113.78	110.43
14	A6	1620	CLA	C4A-NA-C1A	2.71	109.81	106.32
16	A4	849	BCR	C37-C22-C23	2.71	122.41	118.10
16	A1	842	BCR	C37-C22-C23	2.71	122.41	118.10
14	A2	1632	CLA	C3C-C4C-NC	2.71	113.78	110.43
14	A5	804	CLA	C3C-C4C-NC	2.71	113.78	110.43
16	A1	846	BCR	C2-C1-C6	2.71	114.71	110.48
16	L3	206	BCR	C36-C18-C19	2.71	122.41	118.10
14	B1	814	CLA	CMB-C2B-C3B	2.71	129.81	124.88
14	B1	823	CLA	C2C-C1C-NC	2.71	112.89	110.09
14	A6	1614	CLA	C2C-C1C-NC	2.71	112.90	110.09
16	M2	1202	BCR	C37-C22-C23	2.71	122.42	118.10
14	A5	833	CLA	O2A-CGA-CBA	2.71	119.76	111.92
14	A3	811	CLA	C3C-C4C-NC	2.71	113.78	110.43
16	B1	848	BCR	C34-C9-C8	2.71	122.42	118.10
14	B3	1802	CLA	CMB-C2B-C3B	2.71	129.82	124.88
14	A1	813	CLA	CED-O2D-CGD	2.71	122.22	115.97
14	B6	803	CLA	CED-O2D-CGD	2.71	122.22	115.97
14	A2	1608	CLA	CBA-CAA-C2A	2.71	121.86	113.82
14	B5	1820	CLA	CED-O2D-CGD	2.71	122.22	115.97
14	B3	1837	CLA	C3C-C4C-NC	2.71	113.79	110.43
14	X5	101	CLA	C2C-C1C-NC	2.71	112.90	110.09
14	L2	202	CLA	O2A-CGA-CBA	2.71	119.77	111.92
14	L5	203	CLA	O2A-CGA-CBA	2.71	119.77	111.92
14	L2	207	CLA	C3C-C4C-NC	2.71	113.79	110.43
14	B6	808	CLA	C3C-C4C-NC	2.71	113.79	110.43
14	A1	833	CLA	CED-O2D-CGD	2.71	122.23	115.97
14	A1	810	CLA	O2D-CGD-CBD	2.72	116.10	111.28
14	A6	1633	CLA	O2A-CGA-CBA	2.72	119.77	111.92
14	B3	1805	CLA	C2C-C1C-NC	2.72	112.90	110.09
14	B2	824	CLA	CMB-C2B-C3B	2.72	129.83	124.88
14	B6	825	CLA	CMB-C2B-C3B	2.72	129.83	124.88
16	B2	847	BCR	C29-C30-C25	2.72	114.73	110.48
14	L5	206	CLA	C3C-C4C-NC	2.72	113.79	110.43
14	B4	807	CLA	C3B-C4B-NB	2.72	112.72	109.21
14	A4	832	CLA	C3B-C4B-NB	2.72	112.72	109.21
14	A6	1621	CLA	CED-O2D-CGD	2.72	122.23	115.97
14	B6	815	CLA	C2C-C1C-NC	2.72	112.91	110.09
16	J6	1105	BCR	C30-C25-C24	2.72	123.37	115.73
14	A6	1606	CLA	CBA-CAA-C2A	2.72	121.89	113.82
16	A6	1643	BCR	C37-C22-C23	2.72	122.43	118.10
14	L5	204	CLA	C3C-C4C-NC	2.72	113.80	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	809	CLA	C3C-C4C-NC	2.72	113.80	110.43
14	B3	1803	CLA	C3C-C4C-NC	2.72	113.80	110.43
14	L2	206	CLA	C2C-C1C-NC	2.72	112.91	110.09
14	A4	802	CLA	C2C-C1C-NC	2.72	112.91	110.09
14	A3	817	CLA	C3C-C4C-NC	2.73	113.80	110.43
14	L1	201	CLA	C4A-NA-C1A	2.73	109.84	106.32
16	J5	103	BCR	C32-C1-C6	2.73	114.73	110.31
16	I4	102	BCR	C37-C22-C23	2.73	122.44	118.10
14	F1	1301	CLA	C3C-C4C-NC	2.73	113.80	110.43
14	L1	202	CLA	C3C-C4C-NC	2.73	113.80	110.43
14	B5	1807	CLA	C3B-C4B-NB	2.73	112.74	109.21
14	B1	840	CLA	C3C-C4C-NC	2.73	113.81	110.43
14	B5	1817	CLA	C2C-C1C-NC	2.73	112.91	110.09
16	B5	1850	BCR	C34-C9-C8	2.73	122.45	118.10
16	L6	204	BCR	C37-C22-C23	2.73	122.45	118.10
14	A6	1632	CLA	C3B-C4B-NB	2.73	112.74	109.21
14	A3	806	CLA	CBA-CAA-C2A	2.73	121.92	113.82
14	B5	1828	CLA	C3C-C4C-NC	2.73	113.81	110.43
14	A6	1616	CLA	C3C-C4C-NC	2.73	113.81	110.43
14	A1	833	CLA	C2C-C1C-NC	2.73	112.92	110.09
14	B1	841	CLA	C3C-C4C-NC	2.73	113.81	110.43
16	I3	102	BCR	C37-C22-C23	2.73	122.45	118.10
14	A1	804	CLA	C2C-C1C-NC	2.73	112.92	110.09
14	B1	836	CLA	O2D-CGD-CBD	2.73	116.13	111.28
14	B4	839	CLA	C2C-C1C-NC	2.74	112.92	110.09
14	B1	803	CLA	CED-O2D-CGD	2.74	122.27	115.97
16	B6	847	BCR	C36-C18-C19	2.74	122.46	118.10
14	A2	1634	CLA	C4A-NA-C1A	2.74	109.85	106.32
14	B2	834	CLA	O2D-CGD-CBD	2.74	116.13	111.28
14	B6	837	CLA	O2A-CGA-CBA	2.74	119.83	111.92
14	A5	816	CLA	C3C-C4C-NC	2.74	113.82	110.43
16	B2	845	BCR	C40-C30-C25	2.74	114.75	110.31
16	A3	847	BCR	C37-C22-C23	2.74	122.46	118.10
14	B3	1810	CLA	C3C-C4C-NC	2.74	113.82	110.43
14	A4	816	CLA	C3C-C4C-NC	2.74	113.82	110.43
14	B5	1837	CLA	C3C-C4C-NC	2.74	113.82	110.43
14	A2	1635	CLA	O2A-CGA-CBA	2.74	119.84	111.92
14	A2	1636	CLA	C2C-C1C-NC	2.74	112.93	110.09
16	I2	101	BCR	C36-C18-C19	2.74	122.47	118.10
14	B3	1833	CLA	O2A-CGA-CBA	2.74	119.84	111.92
14	A2	1638	CLA	C3B-C4B-NB	2.74	112.75	109.21
14	A2	1628	CLA	C3C-C4C-NC	2.74	113.82	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A1	827	CLA	CMB-C2B-C3B	2.74	129.87	124.88
14	B1	825	CLA	CED-O2D-CGD	2.74	122.29	115.97
14	B2	819	CLA	C2C-C1C-NC	2.74	112.93	110.09
14	B6	832	CLA	C2C-C1C-NC	2.74	112.93	110.09
14	A3	829	CLA	C3C-C4C-NC	2.74	113.82	110.43
16	A4	844	BCR	C37-C22-C23	2.74	122.47	118.10
16	F4	204	BCR	C38-C26-C25	2.74	127.58	124.51
14	A2	1616	CLA	C2C-C1C-NC	2.74	112.93	110.09
14	A3	808	CLA	C3C-C4C-NC	2.75	113.83	110.43
14	B1	853	CLA	C3C-C4C-NC	2.75	113.83	110.43
14	A1	816	CLA	C3C-C4C-NC	2.75	113.83	110.43
14	A5	821	CLA	C2C-C1C-NC	2.75	112.93	110.09
14	A4	853	CLA	C2C-C1C-NC	2.75	112.93	110.09
16	A4	845	BCR	C29-C30-C25	2.75	114.77	110.48
14	A3	845	CLA	C3C-C4C-NC	2.75	113.83	110.43
16	B1	846	BCR	C40-C30-C25	2.75	114.77	110.31
14	A6	1626	CLA	O2A-CGA-CBA	2.75	119.87	111.92
14	B1	803	CLA	O2D-CGD-CBD	2.75	116.16	111.28
16	I6	102	BCR	C36-C18-C19	2.75	122.48	118.10
14	A6	1607	CLA	C3C-C4C-NC	2.75	113.83	110.43
14	L2	205	CLA	C2C-C1C-NC	2.75	112.94	110.09
14	A6	1621	CLA	O2D-CGD-CBD	2.75	116.16	111.28
14	B3	1831	CLA	C3B-C4B-NB	2.75	112.77	109.21
16	B6	846	BCR	C40-C30-C25	2.75	114.77	110.31
14	A3	814	CLA	C2C-C1C-NC	2.75	112.94	110.09
14	B6	816	CLA	C2C-C1C-NC	2.75	112.94	110.09
14	B4	837	CLA	C3C-C4C-NC	2.76	113.84	110.43
14	L5	203	CLA	C3C-C4C-NC	2.76	113.84	110.43
14	B4	834	CLA	C2C-C1C-NC	2.76	112.94	110.09
16	A4	848	BCR	C2-C1-C6	2.76	114.79	110.48
14	B6	819	CLA	C3C-C4C-NC	2.76	113.84	110.43
14	F6	202	CLA	CED-O2D-CGD	2.76	122.33	115.97
16	L5	201	BCR	C29-C30-C25	2.76	114.79	110.48
14	L1	205	CLA	C2C-C1C-NC	2.76	112.95	110.09
14	B1	830	CLA	C3B-C4B-NB	2.76	112.78	109.21
14	B5	1827	CLA	CMB-C2B-C3B	2.76	129.91	124.88
16	I6	102	BCR	C29-C30-C25	2.76	114.80	110.48
14	A5	820	CLA	C4A-NA-C1A	2.76	109.89	106.32
14	B6	835	CLA	O2D-CGD-CBD	2.76	116.18	111.28
14	A4	831	CLA	C3C-C4C-NC	2.76	113.85	110.43
14	B2	815	CLA	C2C-C1C-NC	2.76	112.95	110.09
14	B5	1842	CLA	C3C-C4C-NC	2.76	113.85	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	839	CLA	C3C-C4C-NC	2.76	113.85	110.43
14	B6	835	CLA	C3C-C4C-NC	2.77	113.85	110.43
14	A1	839	CLA	C3C-C4C-NC	2.77	113.85	110.43
16	J5	104	BCR	C30-C25-C24	2.77	123.50	115.73
14	B4	820	CLA	CED-O2D-CGD	2.77	122.35	115.97
14	B6	830	CLA	C2C-C1C-NC	2.77	112.96	110.09
14	B2	808	CLA	C3C-C4C-NC	2.77	113.86	110.43
14	B6	805	CLA	C2C-C1C-NC	2.77	112.96	110.09
14	L1	202	CLA	O2A-CGA-CBA	2.77	119.93	111.92
16	F4	201	BCR	C34-C9-C8	2.77	122.51	118.10
14	A4	804	CLA	C2C-C1C-NC	2.77	112.96	110.09
14	B4	828	CLA	CMB-C2B-C3B	2.77	129.93	124.88
14	B3	1821	CLA	C3C-C4C-NC	2.77	113.86	110.43
14	A1	832	CLA	C2C-C1C-NC	2.77	112.96	110.09
14	B1	826	CLA	CMB-C2B-C3B	2.77	129.93	124.88
14	B2	837	CLA	CED-O2D-CGD	2.77	122.36	115.97
16	I3	101	BCR	C36-C18-C19	2.77	122.52	118.10
16	L5	201	BCR	C38-C26-C25	2.77	127.61	124.51
14	A2	1631	CLA	C3C-C4C-NC	2.77	113.86	110.43
14	B4	811	CLA	C3C-C4C-NC	2.77	113.86	110.43
14	B5	1825	CLA	C2C-C1C-NC	2.77	112.96	110.09
14	B6	829	CLA	C3B-C4B-NB	2.77	112.80	109.21
14	A1	813	CLA	C2C-C1C-NC	2.77	112.96	110.09
14	B5	1834	CLA	C2C-C1C-NC	2.77	112.96	110.09
14	A2	1622	CLA	C4A-NA-C1A	2.78	109.90	106.32
14	B6	817	CLA	C2C-C1C-NC	2.78	112.97	110.09
14	A3	824	CLA	O2A-CGA-CBA	2.78	119.95	111.92
14	B4	827	CLA	CMB-C2B-C3B	2.78	129.94	124.88
14	L6	203	CLA	C3C-C4C-NC	2.78	113.87	110.43
14	A5	828	CLA	CMB-C2B-C3B	2.78	129.94	124.88
14	B5	1830	CLA	O2D-CGD-CBD	2.78	116.21	111.28
16	J5	105	BCR	C38-C26-C25	2.78	127.62	124.51
14	B4	819	CLA	C2C-C1C-NC	2.78	112.97	110.09
14	B1	810	CLA	C3C-C4C-NC	2.78	113.87	110.43
14	B5	1813	CLA	C2C-C1C-NC	2.78	112.97	110.09
14	A6	1611	CLA	O2D-CGD-CBD	2.78	116.21	111.28
14	B3	1815	CLA	CAC-C3C-C4C	2.78	128.66	124.82
14	A2	1617	CLA	C2C-C1C-NC	2.78	112.97	110.09
14	B6	811	CLA	C2C-C1C-NC	2.78	112.97	110.09
16	L2	203	BCR	C33-C5-C6	2.78	127.62	124.51
14	L1	206	CLA	O2A-CGA-CBA	2.78	119.97	111.92
14	A3	834	CLA	O2A-CGA-CBA	2.78	119.97	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L2	206	CLA	O2A-CGA-CBA	2.78	119.97	111.92
14	A1	819	CLA	C4A-NA-C1A	2.78	109.91	106.32
14	B5	1803	CLA	CED-O2D-CGD	2.78	122.39	115.97
14	A2	1610	CLA	C3C-C4C-NC	2.78	113.88	110.43
14	L5	206	CLA	O2A-CGA-CBA	2.78	119.97	111.92
14	A6	1615	CLA	C2C-C1C-NC	2.79	112.97	110.09
14	A3	840	CLA	CED-O2D-CGD	2.79	122.39	115.97
14	B4	822	CLA	C4A-NA-C1A	2.79	109.92	106.32
16	A1	843	BCR	C32-C1-C6	2.79	114.83	110.31
14	B2	840	CLA	C3C-C4C-NC	2.79	113.88	110.43
14	B5	1805	CLA	C2C-C1C-NC	2.79	112.98	110.09
16	J4	104	BCR	C30-C25-C24	2.79	123.57	115.73
14	A4	814	CLA	C2C-C1C-NC	2.79	112.98	110.09
16	A5	853	BCR	C29-C30-C25	2.79	114.84	110.48
16	B1	852	BCR	C38-C26-C25	2.79	127.63	124.51
14	L6	206	CLA	C2C-C1C-NC	2.79	112.98	110.09
14	B2	812	CLA	CMB-C2B-C3B	2.79	129.97	124.88
14	A4	827	CLA	CMB-C2B-C3B	2.79	129.97	124.88
14	A2	1630	CLA	CMB-C2B-C3B	2.79	129.97	124.88
14	A6	1602	CLA	C3C-C4C-NC	2.79	113.89	110.43
14	B4	832	CLA	C2C-C1C-NC	2.80	112.98	110.09
14	A3	815	CLA	C2C-C1C-NC	2.80	112.98	110.09
14	A6	1601	CLA	C2C-C1C-NC	2.80	112.98	110.09
14	B3	1811	CLA	C3C-C4C-NC	2.80	113.89	110.43
16	A3	848	BCR	C29-C30-C25	2.80	114.85	110.48
14	F2	204	CLA	C2C-C1C-NC	2.80	112.99	110.09
14	A5	836	CLA	C3B-C4B-NB	2.80	112.83	109.21
16	L2	201	BCR	C29-C30-C25	2.80	114.86	110.48
14	B3	1825	CLA	C2C-C1C-NC	2.80	112.99	110.09
14	B1	829	CLA	O2D-CGD-CBD	2.80	116.25	111.28
14	L2	205	CLA	C3C-C4C-NC	2.80	113.90	110.43
14	A3	816	CLA	C3C-C4C-NC	2.80	113.90	110.43
14	J6	1103	CLA	C2C-C1C-NC	2.80	112.99	110.09
14	A1	834	CLA	C3C-C4C-NC	2.80	113.90	110.43
16	B1	849	BCR	C29-C30-C25	2.80	114.86	110.48
14	A3	828	CLA	CMB-C2B-C3B	2.80	129.98	124.88
14	B1	830	CLA	O2A-CGA-CBA	2.80	120.03	111.92
14	B6	818	CLA	CED-O2D-CGD	2.81	122.44	115.97
14	A3	832	CLA	C4A-NA-C1A	2.81	109.94	106.32
14	A5	814	CLA	C2C-C1C-NC	2.81	113.00	110.09
14	A3	835	CLA	C2C-C1C-NC	2.81	113.00	110.09
14	A3	833	CLA	C3B-C4B-NB	2.81	112.84	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A4	823	CLA	O2A-CGA-CBA	2.81	120.04	111.92
14	A5	834	CLA	C2C-C1C-NC	2.81	113.00	110.09
14	B3	1828	CLA	C2C-C1C-NC	2.81	113.00	110.09
16	M2	1202	BCR	C29-C30-C25	2.81	114.87	110.48
14	B4	802	CLA	C1-O2A-CGA	2.81	123.24	116.77
16	L6	201	BCR	C38-C26-C25	2.81	127.65	124.51
14	B4	821	CLA	C3C-C4C-NC	2.81	113.91	110.43
14	A3	821	CLA	CED-O2D-CGD	2.81	122.45	115.97
14	B6	815	CLA	C3C-C4C-NC	2.81	113.91	110.43
14	A5	842	CLA	C3C-C4C-NC	2.81	113.91	110.43
16	B6	846	BCR	C29-C30-C25	2.81	114.88	110.48
14	B5	1833	CLA	O2A-CGA-CBA	2.81	120.06	111.92
14	B6	826	CLA	C2C-C1C-NC	2.81	113.00	110.09
16	B3	1849	BCR	C40-C30-C25	2.82	114.87	110.31
14	A2	1628	CLA	CMB-C2B-C3B	2.82	130.01	124.88
14	B5	1837	CLA	O2D-CGD-CBD	2.82	116.28	111.28
16	A6	1644	BCR	C32-C1-C6	2.82	114.88	110.31
16	I5	102	BCR	C33-C5-C6	2.82	127.66	124.51
14	B4	816	CLA	O2A-CGA-CBA	2.82	120.06	111.92
14	A5	808	CLA	C3C-C4C-NC	2.82	113.92	110.43
14	B2	822	CLA	C2C-C1C-NC	2.82	113.01	110.09
14	A5	821	CLA	CED-O2D-CGD	2.82	122.46	115.97
14	L1	201	CLA	O2A-CGA-CBA	2.82	120.07	111.92
14	B2	803	CLA	C2C-C1C-NC	2.82	113.01	110.09
14	A5	817	CLA	O2A-CGA-CBA	2.82	120.07	111.92
16	L2	203	BCR	C37-C22-C23	2.82	122.59	118.10
14	A3	811	CLA	O2D-CGD-CBD	2.82	116.28	111.28
14	B3	1807	CLA	C3B-C4B-NB	2.82	112.86	109.21
14	B6	823	CLA	C2C-C1C-NC	2.82	113.01	110.09
14	L4	205	CLA	C3C-C4C-NC	2.82	113.92	110.43
14	B3	1829	CLA	CMC-C2C-C1C	2.82	129.38	125.05
14	A6	1629	CLA	C3C-C4C-NC	2.82	113.92	110.43
14	B4	813	CLA	C2C-C1C-NC	2.82	113.01	110.09
14	A2	1601	CLA	C2C-C1C-NC	2.82	113.01	110.09
16	J3	104	BCR	C30-C25-C24	2.82	123.66	115.73
14	A2	1630	CLA	C3C-C4C-NC	2.82	113.92	110.43
14	A5	817	CLA	C3C-C4C-NC	2.82	113.92	110.43
14	J4	102	CLA	C2C-C1C-NC	2.82	113.01	110.09
16	L1	203	BCR	C33-C5-C6	2.82	127.67	124.51
14	A2	1604	CLA	C1-O2A-CGA	2.82	123.28	116.77
14	A2	1637	CLA	C2C-C1C-NC	2.82	113.01	110.09
14	A6	1634	CLA	C2C-C1C-NC	2.83	113.02	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	821	CLA	C4A-NA-C1A	2.83	109.97	106.32
16	B2	846	BCR	C40-C30-C25	2.83	114.89	110.31
16	I4	101	BCR	C36-C18-C19	2.83	122.60	118.10
14	A3	806	CLA	CMB-C2B-C3B	2.83	130.03	124.88
16	J1	104	BCR	C30-C25-C24	2.83	123.67	115.73
14	B6	826	CLA	C3C-C4C-NC	2.83	113.93	110.43
14	B1	827	CLA	C3C-C4C-NC	2.83	113.93	110.43
14	A6	1608	CLA	C3C-C4C-NC	2.83	113.93	110.43
16	J4	104	BCR	C40-C30-C25	2.83	114.90	110.31
14	A5	829	CLA	C3C-C4C-NC	2.83	113.93	110.43
14	B6	814	CLA	O2A-CGA-CBA	2.83	120.10	111.92
14	B5	1824	CLA	C2C-C1C-NC	2.83	113.02	110.09
16	B2	845	BCR	C29-C30-C25	2.83	114.91	110.48
14	B3	1831	CLA	O2A-CGA-CBA	2.83	120.11	111.92
14	A3	837	CLA	C3C-C4C-NC	2.83	113.94	110.43
14	L5	204	CLA	C2C-C1C-NC	2.83	113.02	110.09
14	A2	1626	CLA	O2A-CGA-CBA	2.83	120.11	111.92
16	L6	201	BCR	C29-C30-C25	2.83	114.91	110.48
14	B6	813	CLA	CMB-C2B-C3B	2.83	130.04	124.88
14	B3	1814	CLA	C2C-C1C-NC	2.83	113.03	110.09
14	A2	1641	CLA	CED-O2D-CGD	2.84	122.50	115.97
14	A6	1617	CLA	C3C-C4C-NC	2.84	113.94	110.43
14	B4	815	CLA	C3C-C4C-NC	2.84	113.94	110.43
16	J2	103	BCR	C30-C25-C24	2.84	123.70	115.73
14	B1	802	CLA	C1-O2A-CGA	2.84	123.31	116.77
14	B3	1827	CLA	CMB-C2B-C3B	2.84	130.05	124.88
14	A2	1604	CLA	CED-O2D-CGD	2.84	122.51	115.97
14	L1	207	CLA	C3C-C4C-NC	2.84	113.94	110.43
16	I1	103	BCR	C2-C1-C6	2.84	114.92	110.48
14	A6	1624	CLA	O2A-CGA-CBA	2.84	120.13	111.92
14	A5	843	CLA	C3C-C4C-NC	2.84	113.95	110.43
14	A4	835	CLA	C3C-C4C-NC	2.84	113.95	110.43
14	B4	815	CLA	CMB-C2B-C3B	2.84	130.06	124.88
14	B6	831	CLA	O2A-CGA-CBA	2.84	120.14	111.92
14	B4	824	CLA	C2C-C1C-NC	2.84	113.03	110.09
14	A6	1605	CLA	C2C-C1C-NC	2.84	113.03	110.09
14	A4	825	CLA	C3C-C4C-NC	2.84	113.95	110.43
14	B4	817	CLA	C2C-C1C-NC	2.85	113.04	110.09
14	B5	1842	CLA	CED-O2D-CGD	2.85	122.53	115.97
16	L6	209	BCR	C2-C1-C6	2.85	114.93	110.48
14	B5	1828	CLA	CMB-C2B-C3B	2.85	130.06	124.88
16	M1	1202	BCR	C29-C30-C25	2.85	114.93	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B3	1816	CLA	O2A-CGA-CBA	2.85	120.16	111.92
14	A4	810	CLA	O2D-CGD-CBD	2.85	116.33	111.28
16	A2	1649	BCR	C33-C5-C6	2.85	127.70	124.51
14	A1	823	CLA	O2A-CGA-CBA	2.85	120.16	111.92
14	L4	205	CLA	O2A-CGA-CBA	2.85	120.16	111.92
16	A1	846	BCR	C37-C22-C23	2.85	122.64	118.10
14	B3	1832	CLA	C2C-C1C-NC	2.85	113.04	110.09
14	A6	1635	CLA	C2C-C1C-NC	2.85	113.04	110.09
14	B1	832	CLA	O2A-CGA-CBA	2.85	120.17	111.92
16	B1	846	BCR	C29-C30-C25	2.85	114.94	110.48
14	B1	841	CLA	O2A-CGA-CBA	2.85	120.17	111.92
14	B2	817	CLA	CED-O2D-CGD	2.85	122.55	115.97
14	A3	807	CLA	C3C-C4C-NC	2.86	113.96	110.43
14	A5	824	CLA	O2A-CGA-CBA	2.86	120.18	111.92
14	B6	833	CLA	C2C-C1C-NC	2.86	113.05	110.09
14	A3	826	CLA	CMB-C2B-C3B	2.86	130.08	124.88
14	A4	825	CLA	CMB-C2B-C3B	2.86	130.08	124.88
16	L2	208	BCR	C2-C1-C6	2.86	114.94	110.48
16	J3	104	BCR	C40-C30-C25	2.86	114.94	110.31
14	A5	828	CLA	C3C-C4C-NC	2.86	113.97	110.43
14	A6	1626	CLA	C3C-C4C-NC	2.86	113.97	110.43
16	A3	848	BCR	C32-C1-C6	2.86	114.94	110.31
14	L3	204	CLA	O2A-CGA-CBA	2.86	120.18	111.92
14	A4	835	CLA	C3B-C4B-NB	2.86	112.91	109.21
14	A5	815	CLA	C2C-C1C-NC	2.86	113.05	110.09
14	L4	203	CLA	C2C-C1C-NC	2.86	113.05	110.09
14	B2	813	CLA	O2A-CGA-CBA	2.86	120.19	111.92
16	A5	849	BCR	C37-C22-C23	2.86	122.66	118.10
14	L5	205	CLA	O2A-CGA-CBA	2.86	120.19	111.92
14	B4	833	CLA	O2A-CGA-CBA	2.86	120.19	111.92
14	B3	1843	CLA	O2A-CGA-CBA	2.86	120.19	111.92
14	B1	818	CLA	C2C-C1C-NC	2.86	113.05	110.09
14	A2	1634	CLA	O2A-CGA-CBA	2.86	120.19	111.92
14	B3	1813	CLA	C2C-C1C-NC	2.86	113.05	110.09
14	J1	102	CLA	C2C-C1C-NC	2.86	113.05	110.09
14	B5	1817	CLA	C3C-C4C-NC	2.86	113.97	110.43
14	A1	837	CLA	C3C-C4C-NC	2.86	113.97	110.43
14	A5	832	CLA	O2A-CGA-CBA	2.86	120.20	111.92
14	B2	825	CLA	CMB-C2B-C3B	2.86	130.09	124.88
16	L4	206	BCR	C2-C1-C6	2.86	114.96	110.48
14	A5	826	CLA	C3C-C4C-NC	2.86	113.97	110.43
14	A5	801	CLA	OBD-CAD-C3D	2.86	133.31	128.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1808	CLA	O2D-CGD-CBD	2.87	116.36	111.28
14	B3	1822	CLA	C4A-NA-C1A	2.87	110.02	106.32
14	B1	816	CLA	C3C-C4C-NC	2.87	113.98	110.43
14	A2	1638	CLA	C3C-C4C-NC	2.87	113.98	110.43
14	B4	801	CLA	C3C-C4C-NC	2.87	113.98	110.43
16	B5	1845	BCR	C29-C30-C25	2.87	114.96	110.48
14	A5	805	CLA	C2C-C1C-NC	2.87	113.06	110.09
14	B3	1824	CLA	C2C-C1C-NC	2.87	113.06	110.09
14	A3	801	CLA	OBD-CAD-C3D	2.87	133.32	128.09
14	A5	836	CLA	C3C-C4C-NC	2.87	113.98	110.43
14	A1	807	CLA	C3C-C4C-NC	2.87	113.98	110.43
16	L3	206	BCR	C2-C1-C6	2.87	114.97	110.48
16	J5	104	BCR	C40-C30-C25	2.87	114.97	110.31
14	B3	1815	CLA	CMB-C2B-C3B	2.87	130.11	124.88
14	B5	1811	CLA	C3C-C4C-NC	2.87	113.98	110.43
14	A6	1628	CLA	C3C-C4C-NC	2.87	113.99	110.43
14	B3	1815	CLA	C3C-C4C-NC	2.87	113.99	110.43
14	A2	1636	CLA	O2A-CGA-CBA	2.87	120.23	111.92
14	A5	802	CLA	C3C-C4C-NC	2.87	113.99	110.43
14	A1	834	CLA	C3B-C4B-NB	2.88	112.93	109.21
14	B5	1819	CLA	C2C-C1C-NC	2.88	113.07	110.09
14	A6	1636	CLA	C3C-C4C-NC	2.88	113.99	110.43
14	A4	834	CLA	C2C-C1C-NC	2.88	113.07	110.09
16	A6	1646	BCR	C29-C30-C25	2.88	114.97	110.48
14	A1	825	CLA	C3C-C4C-NC	2.88	113.99	110.43
16	A4	846	BCR	C33-C5-C6	2.88	127.73	124.51
14	B2	818	CLA	C3C-C4C-NC	2.88	113.99	110.43
14	B6	841	CLA	O2A-CGA-CBA	2.88	120.24	111.92
16	L6	204	BCR	C33-C5-C6	2.88	127.73	124.51
16	L4	208	BCR	C29-C30-C25	2.88	114.98	110.48
14	A1	825	CLA	CMB-C2B-C3B	2.88	130.12	124.88
14	A3	842	CLA	C3C-C4C-NC	2.88	113.99	110.43
14	A1	806	CLA	C3C-C4C-NC	2.88	113.99	110.43
16	J6	1105	BCR	C40-C30-C25	2.88	114.97	110.31
14	I1	101	CLA	CED-O2D-CGD	2.88	122.60	115.97
14	A4	807	CLA	C3C-C4C-NC	2.88	113.99	110.43
14	A3	836	CLA	C2C-C1C-NC	2.88	113.07	110.09
14	A4	831	CLA	O2A-CGA-CBA	2.88	120.25	111.92
14	B1	820	CLA	C3C-C4C-NC	2.88	113.99	110.43
16	A3	848	BCR	C40-C30-C25	2.88	114.98	110.31
16	A6	1647	BCR	C37-C22-C23	2.88	122.69	118.10
14	L3	202	CLA	C2C-C1C-NC	2.88	113.08	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A2	1619	CLA	O2A-CGA-CBA	2.88	120.26	111.92
14	J3	102	CLA	C2C-C1C-NC	2.88	113.08	110.09
14	B6	840	CLA	CED-O2D-CGD	2.89	122.62	115.97
14	B2	839	CLA	CED-O2D-CGD	2.89	122.62	115.97
14	B4	818	CLA	C2C-C1C-NC	2.89	113.08	110.09
14	B6	822	CLA	C2C-C1C-NC	2.89	113.08	110.09
14	B3	1834	CLA	C2C-C1C-NC	2.89	113.08	110.09
16	A5	846	BCR	C32-C1-C6	2.89	114.99	110.31
14	B4	831	CLA	O2A-CGA-CBA	2.89	120.27	111.92
14	A1	814	CLA	C2C-C1C-NC	2.89	113.08	110.09
14	B1	817	CLA	C2C-C1C-NC	2.89	113.08	110.09
14	A1	805	CLA	CMB-C2B-C3B	2.89	130.14	124.88
16	I5	101	BCR	C36-C18-C19	2.89	122.70	118.10
14	K6	1401	CLA	C2C-C1C-NC	2.89	113.08	110.09
14	B6	802	CLA	C3C-C4C-NC	2.89	114.01	110.43
14	A1	828	CLA	C3C-C4C-NC	2.89	114.01	110.43
16	I5	101	BCR	C33-C5-C6	2.89	127.75	124.51
14	B2	811	CLA	C2C-C1C-NC	2.89	113.09	110.09
14	B5	1814	CLA	C2C-C1C-NC	2.89	113.09	110.09
14	B3	1828	CLA	C3C-C4C-NC	2.89	114.01	110.43
14	B3	1806	CLA	C2C-C1C-NC	2.90	113.09	110.09
14	B2	825	CLA	C2C-C1C-NC	2.90	113.09	110.09
14	B4	843	CLA	O2A-CGA-CBA	2.90	120.30	111.92
16	L1	203	BCR	C37-C22-C23	2.90	122.72	118.10
16	M5	101	BCR	C29-C30-C25	2.90	115.01	110.48
14	L5	202	CLA	C2C-C1C-NC	2.90	113.09	110.09
14	A6	1617	CLA	C2C-C1C-NC	2.90	113.09	110.09
14	B4	825	CLA	C2C-C1C-NC	2.90	113.09	110.09
14	A3	802	CLA	C3C-C4C-NC	2.90	114.02	110.43
14	L6	202	CLA	O2A-CGA-CBA	2.90	120.30	111.92
14	B5	1831	CLA	O2A-CGA-CBA	2.90	120.31	111.92
14	B2	830	CLA	O2A-CGA-CBA	2.90	120.31	111.92
16	A3	851	BCR	C37-C22-C23	2.90	122.72	118.10
14	B4	803	CLA	CED-O2D-CGD	2.90	122.66	115.97
14	B1	827	CLA	CMB-C2B-C3B	2.90	130.17	124.88
14	B2	810	CLA	C2C-C1C-NC	2.90	113.10	110.09
14	A1	816	CLA	O2A-CGA-CBA	2.90	120.31	111.92
14	A2	1633	CLA	O2A-CGA-CBA	2.90	120.32	111.92
14	B4	814	CLA	C2C-C1C-NC	2.91	113.10	110.09
14	L3	205	CLA	C3C-C4C-NC	2.91	114.03	110.43
14	B4	820	CLA	C2C-C1C-NC	2.91	113.10	110.09
14	A4	827	CLA	C3C-C4C-NC	2.91	114.03	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L4	208	BCR	C38-C26-C25	2.91	127.77	124.51
14	B1	824	CLA	C2C-C1C-NC	2.91	113.11	110.09
14	A2	1603	CLA	C3C-C4C-NC	2.91	114.03	110.43
14	B1	819	CLA	C2C-C1C-NC	2.91	113.11	110.09
14	B6	818	CLA	C2C-C1C-NC	2.91	113.11	110.09
16	A5	847	BCR	C33-C5-C6	2.91	127.77	124.51
14	B4	815	CLA	CAC-C3C-C4C	2.92	128.84	124.82
14	B4	841	CLA	O2A-CGA-CBA	2.92	120.35	111.92
14	B3	1830	CLA	O2D-CGD-CBD	2.92	116.45	111.28
16	L5	207	BCR	C2-C1-C6	2.92	115.04	110.48
14	A5	835	CLA	C2C-C1C-NC	2.92	113.11	110.09
14	B6	829	CLA	O2A-CGA-CBA	2.92	120.36	111.92
16	I1	102	BCR	C33-C5-C6	2.92	127.78	124.51
16	B6	847	BCR	C40-C30-C25	2.92	115.04	110.31
14	A2	1628	CLA	C2C-C1C-NC	2.92	113.11	110.09
14	A6	1626	CLA	CMB-C2B-C3B	2.92	130.20	124.88
14	A2	1639	CLA	O2A-CGA-CBA	2.92	120.36	111.92
14	B4	840	CLA	CED-O2D-CGD	2.92	122.70	115.97
14	A3	832	CLA	O2A-CGA-CBA	2.92	120.37	111.92
16	A6	1644	BCR	C40-C30-C25	2.92	115.05	110.31
14	A5	806	CLA	CMB-C2B-C3B	2.92	130.20	124.88
14	A3	817	CLA	C2C-C1C-NC	2.92	113.12	110.09
14	A5	839	CLA	O2D-CGD-CBD	2.92	116.47	111.28
14	A3	826	CLA	C3C-C4C-NC	2.93	114.05	110.43
14	B2	823	CLA	O2A-CGA-CBA	2.93	120.38	111.92
14	A4	830	CLA	O2A-CGA-CBA	2.93	120.39	111.92
14	A6	1606	CLA	CMB-C2B-C3B	2.93	130.21	124.88
16	I6	102	BCR	C33-C5-C6	2.93	127.79	124.51
14	F4	202	CLA	C2C-C1C-NC	2.93	113.12	110.09
14	A5	811	CLA	O2D-CGD-CBD	2.93	116.48	111.28
14	B2	828	CLA	O2A-CGA-CBA	2.93	120.39	111.92
14	A4	804	CLA	O2A-CGA-CBA	2.93	120.39	111.92
16	I1	102	BCR	C36-C18-C19	2.93	122.77	118.10
14	B3	1821	CLA	O2A-CGA-CBA	2.93	120.39	111.92
14	A5	840	CLA	C3C-C4C-NC	2.93	114.06	110.43
14	B2	818	CLA	O2A-CGA-CBA	2.93	120.40	111.92
14	B1	802	CLA	CED-O2D-CGD	2.93	122.73	115.97
14	B3	1817	CLA	C3C-C4C-NC	2.93	114.06	110.43
14	A2	1643	CLA	C3C-C4C-NC	2.93	114.06	110.43
14	A2	1607	CLA	C2C-C1C-NC	2.93	113.13	110.09
14	B5	1843	CLA	O2A-CGA-CBA	2.93	120.40	111.92
14	A2	1607	CLA	O2A-CGA-CBA	2.93	120.40	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	805	CLA	C3C-C4C-NC	2.93	114.06	110.43
16	J5	105	BCR	C29-C30-C25	2.94	115.07	110.48
14	B5	1826	CLA	O2A-CGA-CBA	2.94	120.41	111.92
14	A1	827	CLA	C3C-C4C-NC	2.94	114.06	110.43
14	B4	829	CLA	C2C-C1C-NC	2.94	113.13	110.09
14	A4	828	CLA	C3C-C4C-NC	2.94	114.06	110.43
14	B4	828	CLA	C3C-C4C-NC	2.94	114.06	110.43
14	B1	823	CLA	O2A-CGA-CBA	2.94	120.41	111.92
14	A3	835	CLA	O2A-CGA-CBA	2.94	120.41	111.92
14	A6	1637	CLA	O2A-CGA-CBA	2.94	120.42	111.92
14	B5	1835	CLA	O2A-CGA-CBA	2.94	120.42	111.92
14	F2	202	CLA	C2C-C1C-NC	2.94	113.13	110.09
14	A5	817	CLA	C2C-C1C-NC	2.94	113.13	110.09
14	L2	207	CLA	O2A-CGA-CBA	2.94	120.42	111.92
14	B2	814	CLA	C3C-C4C-NC	2.94	114.07	110.43
14	L6	208	CLA	C3C-C4C-NC	2.94	114.07	110.43
16	A4	848	BCR	C37-C22-C23	2.94	122.79	118.10
14	L3	203	CLA	O2A-CGA-CBA	2.94	120.43	111.92
16	M3	1602	BCR	C29-C30-C25	2.95	115.08	110.48
14	F6	202	CLA	C2C-C1C-NC	2.95	113.14	110.09
14	L1	207	CLA	O2A-CGA-CBA	2.95	120.44	111.92
14	A4	836	CLA	O2D-CGD-CBD	2.95	116.51	111.28
14	B6	827	CLA	C2C-C1C-NC	2.95	113.14	110.09
16	A1	844	BCR	C33-C5-C6	2.95	127.81	124.51
16	M6	1202	BCR	C29-C30-C25	2.95	115.09	110.48
14	A4	816	CLA	C2C-C1C-NC	2.95	113.14	110.09
14	B4	835	CLA	O2A-CGA-CBA	2.95	120.45	111.92
16	B4	848	BCR	C29-C30-C25	2.95	115.09	110.48
14	B3	1818	CLA	C2C-C1C-NC	2.95	113.15	110.09
14	B5	1820	CLA	C2C-C1C-NC	2.95	113.15	110.09
14	A3	831	CLA	O2A-CGA-CBA	2.95	120.46	111.92
16	A2	1652	BCR	C30-C25-C24	2.95	124.03	115.73
14	L4	204	CLA	O2A-CGA-CBA	2.95	120.46	111.92
14	M3	1601	CLA	C2C-C1C-NC	2.95	113.15	110.09
16	I4	101	BCR	C33-C5-C6	2.96	127.82	124.51
14	A3	801	CLA	C3C-C4C-NC	2.96	114.09	110.43
14	A4	839	CLA	C3C-C4C-NC	2.96	114.09	110.43
14	B2	840	CLA	O2A-CGA-CBA	2.96	120.47	111.92
14	B3	1819	CLA	C2C-C1C-NC	2.96	113.15	110.09
14	B5	1822	CLA	C4A-NA-C1A	2.96	110.14	106.32
14	A1	811	CLA	C2C-C1C-NC	2.96	113.16	110.09
14	A4	806	CLA	C3C-C4C-NC	2.96	114.09	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1816	CLA	O2A-CGA-CBA	2.96	120.48	111.92
14	A4	816	CLA	O2A-CGA-CBA	2.96	120.48	111.92
14	B4	817	CLA	C3C-C4C-NC	2.96	114.09	110.43
14	A6	1629	CLA	C2C-C1C-NC	2.96	113.16	110.09
16	A3	852	BCR	C30-C25-C24	2.96	124.06	115.73
14	B2	814	CLA	C2C-C1C-NC	2.96	113.16	110.09
14	B5	1818	CLA	C2C-C1C-NC	2.97	113.16	110.09
14	A3	841	CLA	C3C-C4C-NC	2.97	114.10	110.43
14	L4	203	CLA	O2A-CGA-CBA	2.97	120.50	111.92
14	A4	836	CLA	C2C-C1C-NC	2.97	113.16	110.09
14	A2	1619	CLA	C2C-C1C-NC	2.97	113.16	110.09
14	A5	837	CLA	O2A-CGA-CBA	2.97	120.50	111.92
14	B5	1824	CLA	O2A-CGA-CBA	2.97	120.50	111.92
16	A4	848	BCR	C29-C30-C25	2.97	115.12	110.48
14	B1	808	CLA	O2A-CGA-CBA	2.97	120.50	111.92
14	B5	1803	CLA	O2A-CGA-CBA	2.97	120.50	111.92
14	A1	816	CLA	C2C-C1C-NC	2.97	113.16	110.09
14	B2	821	CLA	C2C-C1C-NC	2.97	113.17	110.09
14	B4	834	CLA	O2A-CGA-CBA	2.97	120.51	111.92
14	B1	804	CLA	CED-O2D-CGD	2.97	122.82	115.97
14	A6	1602	CLA	OBD-CAD-C3D	2.97	133.50	128.09
14	A3	805	CLA	O2A-CGA-CBA	2.97	120.51	111.92
14	A1	835	CLA	O2A-CGA-CBA	2.97	120.52	111.92
14	B1	801	CLA	C3C-C4C-NC	2.97	114.11	110.43
14	B2	825	CLA	C3C-C4C-NC	2.97	114.11	110.43
14	A5	826	CLA	CMB-C2B-C3B	2.97	130.30	124.88
14	A5	805	CLA	O2A-CGA-CBA	2.97	120.52	111.92
14	B6	807	CLA	O2D-CGD-CBD	2.98	116.56	111.28
14	A1	840	CLA	C2C-C1C-NC	2.98	113.17	110.09
16	A5	845	BCR	C33-C5-C6	2.98	127.84	124.51
17	A3	853	LHG	O8-C23-C24	2.98	120.54	111.92
16	L6	209	BCR	C30-C25-C24	2.98	124.11	115.73
14	B1	820	CLA	O2A-CGA-CBA	2.98	120.54	111.92
16	M4	101	BCR	C29-C30-C25	2.98	115.14	110.48
16	B2	850	BCR	C29-C30-C25	2.98	115.14	110.48
14	B5	1815	CLA	C2C-C1C-NC	2.98	113.18	110.09
14	K5	102	CLA	C2C-C1C-NC	2.98	113.18	110.09
16	M2	1202	BCR	C2-C1-C6	2.99	115.14	110.48
14	B1	836	CLA	C2C-C1C-NC	2.99	113.18	110.09
16	B1	852	BCR	C29-C30-C25	2.99	115.15	110.48
14	F5	1301	CLA	C2C-C1C-NC	2.99	113.18	110.09
14	A2	1613	CLA	O2A-CGA-CBA	2.99	120.56	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	804	CLA	O2A-CGA-CBA	2.99	120.56	111.92
14	A6	1640	CLA	C3C-C4C-NC	2.99	114.13	110.43
14	A6	1616	CLA	O2A-CGA-CBA	2.99	120.56	111.92
16	A1	845	BCR	C29-C30-C25	2.99	115.15	110.48
14	B3	1824	CLA	O2A-CGA-CBA	2.99	120.56	111.92
14	A5	834	CLA	O2A-CGA-CBA	2.99	120.56	111.92
14	A6	1617	CLA	O2A-CGA-CBA	2.99	120.56	111.92
17	A1	848	LHG	O7-C7-C8	2.99	117.85	111.55
14	B3	1808	CLA	O2D-CGD-CBD	2.99	116.58	111.28
14	B4	815	CLA	C2C-C1C-NC	2.99	113.19	110.09
14	B1	820	CLA	C2C-C1C-NC	2.99	113.19	110.09
14	A3	807	CLA	C2C-C1C-NC	2.99	113.19	110.09
14	A3	805	CLA	C2C-C1C-NC	2.99	113.19	110.09
14	B1	811	CLA	O2A-CGA-CBA	2.99	120.57	111.92
14	A4	833	CLA	O2A-CGA-CBA	2.99	120.58	111.92
14	A2	1609	CLA	C3C-C4C-NC	3.00	114.14	110.43
16	B6	843	BCR	C29-C30-C25	3.00	115.16	110.48
14	B3	1837	CLA	C2C-C1C-NC	3.00	113.19	110.09
16	I3	102	BCR	C33-C5-C6	3.00	127.86	124.51
14	A1	832	CLA	O2A-CGA-CBA	3.00	120.59	111.92
16	A2	1651	BCR	C37-C22-C23	3.00	122.88	118.10
14	A6	1641	CLA	C2C-C1C-NC	3.00	113.20	110.09
14	A2	1626	CLA	C2C-C1C-NC	3.00	113.20	110.09
14	B1	806	CLA	O2A-CGA-CBA	3.00	120.60	111.92
14	A6	1634	CLA	O2A-CGA-CBA	3.00	120.60	111.92
14	A2	1606	CLA	O2A-CGA-CBA	3.00	120.60	111.92
14	B6	812	CLA	C2C-C1C-NC	3.00	113.20	110.09
16	A2	1651	BCR	C29-C30-C25	3.00	115.17	110.48
14	B4	824	CLA	O2A-CGA-CBA	3.00	120.60	111.92
14	B6	822	CLA	O2A-CGA-CBA	3.00	120.60	111.92
14	A5	841	CLA	C3C-C4C-NC	3.00	114.15	110.43
16	A4	847	BCR	C29-C30-C25	3.00	115.18	110.48
16	L3	206	BCR	C30-C25-C24	3.00	124.17	115.73
14	B5	1821	CLA	C3C-C4C-NC	3.00	114.15	110.43
14	A1	835	CLA	C2C-C1C-NC	3.01	113.20	110.09
14	A6	1611	CLA	O2A-CGA-CBA	3.01	120.61	111.92
14	B3	1820	CLA	C2C-C1C-NC	3.01	113.20	110.09
14	B2	802	CLA	C3C-C4C-NC	3.01	114.15	110.43
14	A6	1605	CLA	O2A-CGA-CBA	3.01	120.62	111.92
14	L6	206	CLA	O2A-CGA-CBA	3.01	120.62	111.92
14	L5	204	CLA	O2A-CGA-CBA	3.01	120.63	111.92
14	A4	836	CLA	O2A-CGA-CBA	3.01	120.63	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A1	804	CLA	O2A-CGA-CBA	3.01	120.63	111.92
14	B2	803	CLA	O2A-CGA-CBA	3.01	120.63	111.92
16	A5	850	BCR	C30-C25-C24	3.01	124.20	115.73
16	A6	1648	BCR	C30-C25-C24	3.01	124.20	115.73
16	B5	1849	BCR	C40-C30-C25	3.01	115.20	110.31
16	M3	1602	BCR	C2-C1-C6	3.01	115.19	110.48
14	A4	840	CLA	C3C-C4C-NC	3.02	114.16	110.43
14	A2	1613	CLA	O2D-CGD-CBD	3.02	116.63	111.28
14	A2	1631	CLA	C2C-C1C-NC	3.02	113.21	110.09
14	B5	1806	CLA	C2C-C1C-NC	3.02	113.21	110.09
14	A1	806	CLA	C2C-C1C-NC	3.02	113.21	110.09
14	A5	807	CLA	C3C-C4C-NC	3.02	114.16	110.43
14	A3	817	CLA	O2A-CGA-CBA	3.02	120.65	111.92
14	B2	827	CLA	O2D-CGD-CBD	3.02	116.64	111.28
16	B3	1845	BCR	C29-C30-C25	3.02	115.20	110.48
16	A4	849	BCR	C30-C25-C24	3.02	124.22	115.73
14	A1	820	CLA	CED-O2D-CGD	3.02	122.93	115.97
14	A4	823	CLA	C2C-C1C-NC	3.02	113.22	110.09
14	A3	804	CLA	O2A-CGA-CBA	3.02	120.66	111.92
14	A1	830	CLA	O2A-CGA-CBA	3.02	120.66	111.92
14	A1	838	CLA	C3C-C4C-NC	3.02	114.17	110.43
16	L2	201	BCR	C38-C26-C25	3.02	127.89	124.51
16	I4	102	BCR	C33-C5-C6	3.02	127.89	124.51
14	A3	829	CLA	C2C-C1C-NC	3.02	113.22	110.09
14	F1	1301	CLA	C2C-C1C-NC	3.02	113.22	110.09
14	A1	836	CLA	C2C-C1C-NC	3.02	113.22	110.09
14	B6	826	CLA	CMB-C2B-C3B	3.02	130.39	124.88
14	A3	828	CLA	C3C-C4C-NC	3.02	114.17	110.43
14	A6	1636	CLA	C3B-C4B-NB	3.02	113.12	109.21
16	B4	845	BCR	C29-C30-C25	3.02	115.21	110.48
14	A3	837	CLA	C3B-C4B-NB	3.03	113.12	109.21
14	M6	1201	CLA	C2C-C1C-NC	3.03	113.22	110.09
14	A3	838	CLA	O2A-CGA-CBA	3.03	120.67	111.92
14	A4	810	CLA	O2A-CGA-CBA	3.03	120.67	111.92
16	B5	1848	BCR	C29-C30-C25	3.03	115.21	110.48
14	A2	1609	CLA	C2C-C1C-NC	3.03	113.22	110.09
16	J6	1104	BCR	C36-C18-C19	3.03	122.92	118.10
14	B3	1826	CLA	O2A-CGA-CBA	3.03	120.68	111.92
14	B6	817	CLA	O2D-CGD-CBD	3.03	116.65	111.28
14	A5	826	CLA	C2C-C1C-NC	3.03	113.23	110.09
16	L2	208	BCR	C30-C25-C24	3.03	124.25	115.73
16	J1	104	BCR	C40-C30-C25	3.03	115.22	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	805	CLA	O2A-CGA-CBA	3.03	120.69	111.92
16	A5	849	BCR	C29-C30-C25	3.03	115.22	110.48
14	A5	804	CLA	O2A-CGA-CBA	3.04	120.70	111.92
14	B3	1811	CLA	O2A-CGA-CBA	3.04	120.70	111.92
14	A3	844	CLA	C2C-C1C-NC	3.04	113.23	110.09
14	K5	101	CLA	C2C-C1C-NC	3.04	113.23	110.09
14	A5	828	CLA	O2D-CGD-CBD	3.04	116.67	111.28
16	B1	843	BCR	C29-C30-C25	3.04	115.22	110.48
16	J3	103	BCR	C36-C18-C19	3.04	122.94	118.10
14	B4	821	CLA	O2A-CGA-CBA	3.04	120.70	111.92
14	A5	811	CLA	O2A-CGA-CBA	3.04	120.70	111.92
14	L3	205	CLA	O2A-CGA-CBA	3.04	120.70	111.92
14	B3	1829	CLA	C2C-C1C-NC	3.04	113.23	110.09
14	B1	814	CLA	C2C-C1C-NC	3.04	113.23	110.09
14	B2	831	CLA	O2A-CGA-CBA	3.04	120.70	111.92
14	A2	1614	CLA	C2C-C1C-NC	3.04	113.24	110.09
14	B6	828	CLA	O2D-CGD-CBD	3.04	116.67	111.28
16	J2	103	BCR	C40-C30-C25	3.04	115.24	110.31
14	A6	1604	CLA	C2C-C1C-NC	3.04	113.24	110.09
14	A1	803	CLA	O2A-CGA-CBA	3.04	120.71	111.92
16	M6	1202	BCR	C2-C1-C6	3.04	115.23	110.48
14	B2	832	CLA	O2A-CGA-CBA	3.04	120.71	111.92
14	A1	810	CLA	O2A-CGA-CBA	3.04	120.71	111.92
14	A6	1612	CLA	C2C-C1C-NC	3.04	113.24	110.09
16	A4	844	BCR	C33-C5-C6	3.04	127.91	124.51
16	L5	207	BCR	C30-C25-C24	3.04	124.28	115.73
16	I3	101	BCR	C33-C5-C6	3.04	127.91	124.51
14	L6	203	CLA	O2D-CGD-CBD	3.04	116.68	111.28
14	A1	828	CLA	C2C-C1C-NC	3.04	113.24	110.09
16	A6	1645	BCR	C33-C5-C6	3.04	127.92	124.51
14	B6	819	CLA	O2A-CGA-CBA	3.05	120.73	111.92
14	A1	815	CLA	O2A-CGA-CBA	3.05	120.73	111.92
14	B1	834	CLA	O2A-CGA-CBA	3.05	120.73	111.92
16	I2	101	BCR	C33-C5-C6	3.05	127.92	124.51
14	K4	1401	CLA	C2C-C1C-NC	3.05	113.25	110.09
14	A5	829	CLA	C2C-C1C-NC	3.05	113.25	110.09
14	F3	202	CLA	C2C-C1C-NC	3.05	113.25	110.09
14	B2	805	CLA	O2D-CGD-CBD	3.05	116.69	111.28
14	A2	1618	CLA	O2A-CGA-CBA	3.05	120.73	111.92
14	A2	1608	CLA	CMB-C2B-C3B	3.05	130.43	124.88
14	B1	815	CLA	O2A-CGA-CBA	3.05	120.74	111.92
14	K1	1401	CLA	C2C-C1C-NC	3.05	113.25	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	809	CLA	O2A-CGA-CBA	3.05	120.74	111.92
14	B6	824	CLA	O2A-CGA-CBA	3.05	120.74	111.92
14	A2	1642	CLA	C3C-C4C-NC	3.05	114.21	110.43
16	A1	846	BCR	C29-C30-C25	3.05	115.25	110.48
14	A4	812	CLA	C2C-C1C-NC	3.05	113.25	110.09
14	A6	1631	CLA	O2A-CGA-CBA	3.05	120.75	111.92
14	A2	1639	CLA	O2D-CGD-CBD	3.05	116.70	111.28
16	I1	103	BCR	C30-C25-C24	3.05	124.31	115.73
14	B3	1802	CLA	C1-O2A-CGA	3.06	123.81	116.77
14	A5	837	CLA	C2C-C1C-NC	3.06	113.25	110.09
16	A1	847	BCR	C30-C25-C24	3.06	124.32	115.73
14	A3	804	CLA	C2C-C1C-NC	3.06	113.26	110.09
14	A6	1607	CLA	C2C-C1C-NC	3.06	113.26	110.09
16	M4	101	BCR	C2-C1-C6	3.06	115.26	110.48
16	A5	846	BCR	C40-C30-C25	3.06	115.27	110.31
14	B5	1802	CLA	C1-O2A-CGA	3.06	123.82	116.77
14	A6	1603	CLA	C1-O2A-CGA	3.06	123.82	116.77
17	A2	1653	LHG	O8-C23-C24	3.06	120.77	111.92
14	B2	808	CLA	O2A-CGA-CBA	3.06	120.77	111.92
14	B6	805	CLA	O2A-CGA-CBA	3.06	120.77	111.92
14	A6	1624	CLA	C2C-C1C-NC	3.06	113.26	110.09
14	B1	813	CLA	C2C-C1C-NC	3.06	113.26	110.09
14	A5	816	CLA	O2A-CGA-CBA	3.06	120.78	111.92
14	A4	803	CLA	O2A-CGA-CBA	3.06	120.78	111.92
14	B3	1803	CLA	O2A-CGA-CBA	3.06	120.78	111.92
14	K2	1401	CLA	C2C-C1C-NC	3.06	113.26	110.09
16	A1	847	BCR	C29-C30-C25	3.06	115.27	110.48
14	B3	1838	CLA	C2C-C1C-NC	3.06	113.26	110.09
14	B1	804	CLA	O2A-CGA-CBA	3.06	120.78	111.92
14	B5	1837	CLA	C2C-C1C-NC	3.07	113.26	110.09
16	F6	203	BCR	C29-C30-C25	3.07	115.27	110.48
17	A4	850	LHG	O8-C23-C24	3.07	120.78	111.92
14	B2	821	CLA	O2A-CGA-CBA	3.07	120.78	111.92
14	A4	806	CLA	C2C-C1C-NC	3.07	113.27	110.09
16	M5	101	BCR	C2-C1-C6	3.07	115.27	110.48
14	A5	813	CLA	C2C-C1C-NC	3.07	113.27	110.09
14	A4	811	CLA	C2C-C1C-NC	3.07	113.27	110.09
14	B2	838	CLA	O2A-CGA-CBA	3.07	120.80	111.92
14	B6	826	CLA	O2A-CGA-CBA	3.07	120.80	111.92
16	F6	201	BCR	C29-C30-C25	3.07	115.28	110.48
14	A3	806	CLA	C2C-C1C-NC	3.07	113.27	110.09
14	A5	812	CLA	C2C-C1C-NC	3.07	113.27	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A4	828	CLA	C2C-C1C-NC	3.07	113.27	110.09
14	A3	812	CLA	C2C-C1C-NC	3.07	113.27	110.09
14	A5	806	CLA	C2C-C1C-NC	3.07	113.27	110.09
16	B5	1845	BCR	C33-C5-C6	3.07	127.95	124.51
16	A5	850	BCR	C29-C30-C25	3.07	115.28	110.48
14	B3	1835	CLA	O2A-CGA-CBA	3.07	120.81	111.92
14	B2	817	CLA	C2C-C1C-NC	3.07	113.27	110.09
14	B5	1821	CLA	O2A-CGA-CBA	3.07	120.81	111.92
16	F4	204	BCR	C29-C30-C25	3.08	115.29	110.48
17	A1	849	LHG	O7-C7-C8	3.08	118.03	111.55
14	A6	1625	CLA	O2A-CGA-CBA	3.08	120.81	111.92
14	A2	1640	CLA	C2C-C1C-NC	3.08	113.28	110.09
14	A4	805	CLA	CMB-C2B-C3B	3.08	130.48	124.88
14	A3	811	CLA	O2A-CGA-CBA	3.08	120.82	111.92
16	B2	842	BCR	C29-C30-C25	3.08	115.29	110.48
14	A6	1639	CLA	C3C-C4C-NC	3.08	114.24	110.43
16	J2	102	BCR	C36-C18-C19	3.08	123.00	118.10
14	B6	813	CLA	O2A-CGA-CBA	3.08	120.83	111.92
14	B5	1805	CLA	O2A-CGA-CBA	3.08	120.83	111.92
14	B2	801	CLA	O2A-CGA-CBA	3.08	120.83	111.92
14	A1	825	CLA	C2C-C1C-NC	3.08	113.28	110.09
14	B6	836	CLA	C2C-C1C-NC	3.08	113.28	110.09
14	B3	1821	CLA	C2C-C1C-NC	3.08	113.28	110.09
14	A4	808	CLA	C2C-C1C-NC	3.08	113.28	110.09
14	A6	1613	CLA	O2A-CGA-CBA	3.08	120.83	111.92
14	A4	815	CLA	O2A-CGA-CBA	3.08	120.84	111.92
14	B3	1819	CLA	O2D-CGD-CBD	3.09	116.75	111.28
14	B4	804	CLA	C3C-C4C-NC	3.09	114.25	110.43
14	L2	205	CLA	O2A-CGA-CBA	3.09	120.84	111.92
16	A3	852	BCR	C29-C30-C25	3.09	115.30	110.48
16	A2	1647	BCR	C33-C5-C6	3.09	127.97	124.51
14	B6	832	CLA	O2A-CGA-CBA	3.09	120.86	111.92
14	L1	205	CLA	O2A-CGA-CBA	3.09	120.86	111.92
16	A5	848	BCR	C29-C30-C25	3.09	115.31	110.48
14	B6	819	CLA	C2C-C1C-NC	3.09	113.29	110.09
14	B4	803	CLA	O2A-CGA-CBA	3.09	120.86	111.92
14	B5	1813	CLA	O2D-CGD-CBD	3.09	116.76	111.28
14	A3	809	CLA	C2C-C1C-NC	3.09	113.29	110.09
14	B6	833	CLA	O2A-CGA-CBA	3.09	120.86	111.92
14	A6	1637	CLA	O2D-CGD-CBD	3.10	116.77	111.28
14	B5	1804	CLA	C3C-C4C-NC	3.10	114.26	110.43
14	A6	1606	CLA	C2C-C1C-NC	3.10	113.30	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	K3	1401	CLA	C2C-C1C-NC	3.10	113.30	110.09
14	B2	818	CLA	C2C-C1C-NC	3.10	113.30	110.09
16	A4	845	BCR	C40-C30-C25	3.10	115.33	110.31
14	B1	840	CLA	O2A-CGA-CBA	3.10	120.88	111.92
14	B5	1815	CLA	O2A-CGA-CBA	3.10	120.88	111.92
14	B5	1834	CLA	O2A-CGA-CBA	3.10	120.88	111.92
14	A2	1645	CLA	C2C-C1C-NC	3.10	113.30	110.09
16	A4	846	BCR	C2-C1-C6	3.10	115.32	110.48
16	F3	203	BCR	C29-C30-C25	3.10	115.33	110.48
16	J5	103	BCR	C36-C18-C19	3.10	123.04	118.10
14	B1	833	CLA	O2A-CGA-CBA	3.10	120.89	111.92
14	A5	824	CLA	C2C-C1C-NC	3.10	113.30	110.09
14	B5	1811	CLA	O2A-CGA-CBA	3.10	120.89	111.92
14	B3	1834	CLA	O2A-CGA-CBA	3.10	120.89	111.92
16	I5	102	BCR	C37-C22-C23	3.10	123.04	118.10
14	B2	826	CLA	C2C-C1C-NC	3.11	113.31	110.09
16	A2	1650	BCR	C29-C30-C25	3.11	115.33	110.48
16	J1	103	BCR	C36-C18-C19	3.11	123.05	118.10
16	B3	1851	BCR	C29-C30-C25	3.11	115.34	110.48
16	A6	1647	BCR	C29-C30-C25	3.11	115.34	110.48
14	B4	816	CLA	C2C-C1C-NC	3.11	113.31	110.09
14	A5	809	CLA	C2C-C1C-NC	3.11	113.31	110.09
14	A1	824	CLA	O2A-CGA-CBA	3.11	120.91	111.92
14	M1	1201	CLA	C2C-C1C-NC	3.11	113.31	110.09
16	M1	1202	BCR	C2-C1-C6	3.11	115.34	110.48
14	A5	831	CLA	O2A-CGA-CBA	3.11	120.92	111.92
14	B3	1828	CLA	CMB-C2B-C3B	3.11	130.55	124.88
14	A3	810	CLA	C2C-C1C-NC	3.11	113.31	110.09
16	L4	206	BCR	C30-C25-C24	3.11	124.48	115.73
16	B3	1845	BCR	C33-C5-C6	3.11	128.00	124.51
14	A5	825	CLA	O2A-CGA-CBA	3.12	120.93	111.92
14	B2	835	CLA	C2C-C1C-NC	3.12	113.32	110.09
14	A2	1644	CLA	O2D-CGD-CBD	3.12	116.81	111.28
14	A6	1651	CLA	C3C-C4C-NC	3.12	114.29	110.43
14	A4	841	CLA	O2D-CGD-CBD	3.12	116.81	111.28
14	A1	808	CLA	C2C-C1C-NC	3.12	113.32	110.09
14	B4	828	CLA	O2A-CGA-CBA	3.12	120.93	111.92
14	B4	826	CLA	O2A-CGA-CBA	3.12	120.94	111.92
16	A3	849	BCR	C2-C1-C6	3.12	115.35	110.48
16	A6	1648	BCR	C29-C30-C25	3.12	115.35	110.48
14	A4	827	CLA	O2A-CGA-CBA	3.12	120.94	111.92
14	A6	1609	CLA	C2C-C1C-NC	3.12	113.32	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A2	1648	BCR	C40-C30-C25	3.12	115.37	110.31
14	B2	813	CLA	C2C-C1C-NC	3.12	113.32	110.09
14	B3	1841	CLA	O2A-CGA-CBA	3.12	120.95	111.92
16	A1	845	BCR	C2-C1-C6	3.12	115.36	110.48
16	L1	209	BCR	C29-C30-C25	3.12	115.36	110.48
14	A2	1639	CLA	C2C-C1C-NC	3.12	113.33	110.09
14	A1	812	CLA	C2C-C1C-NC	3.12	113.33	110.09
14	B5	1807	CLA	O2A-CGA-CBA	3.13	120.96	111.92
14	A4	812	CLA	O2A-CGA-CBA	3.13	120.96	111.92
14	B3	1805	CLA	O2A-CGA-CBA	3.13	120.96	111.92
14	B5	1812	CLA	O2D-CGD-CBD	3.13	116.83	111.28
14	A3	816	CLA	O2A-CGA-CBA	3.13	120.97	111.92
14	B6	835	CLA	C2C-C1C-NC	3.13	113.33	110.09
14	A1	823	CLA	C2C-C1C-NC	3.13	113.33	110.09
14	A1	827	CLA	O2A-CGA-CBA	3.13	120.97	111.92
14	B4	829	CLA	C3C-C4C-NC	3.13	114.30	110.43
14	A6	1613	CLA	C2C-C1C-NC	3.13	113.33	110.09
14	B2	834	CLA	C2C-C1C-NC	3.13	113.33	110.09
14	A1	835	CLA	O2D-CGD-CBD	3.13	116.83	111.28
14	A1	827	CLA	O2D-CGD-CBD	3.13	116.83	111.28
14	A2	1627	CLA	O2A-CGA-CBA	3.13	120.98	111.92
14	A2	1615	CLA	C2C-C1C-NC	3.13	113.33	110.09
16	B6	845	BCR	C33-C5-C6	3.13	128.02	124.51
14	A5	828	CLA	O2A-CGA-CBA	3.13	120.98	111.92
16	A2	1649	BCR	C2-C1-C6	3.14	115.38	110.48
14	B4	830	CLA	O2D-CGD-CBD	3.14	116.85	111.28
14	A4	801	CLA	O2A-CGA-CBA	3.14	121.00	111.92
14	A6	1602	CLA	O2A-CGA-CBA	3.14	121.00	111.92
16	A3	849	BCR	C33-C5-C6	3.14	128.03	124.51
16	A4	844	BCR	C29-C30-C25	3.14	115.39	110.48
14	A3	824	CLA	C2C-C1C-NC	3.14	113.34	110.09
14	B5	1841	CLA	O2A-CGA-CBA	3.14	121.01	111.92
16	B4	845	BCR	C33-C5-C6	3.14	128.03	124.51
14	A2	1630	CLA	O2A-CGA-CBA	3.15	121.02	111.92
14	B4	807	CLA	O2A-CGA-CBA	3.15	121.02	111.92
17	A6	1649	LHG	O8-C23-C24	3.15	121.02	111.92
16	B2	843	BCR	C2-C1-C6	3.15	115.40	110.48
14	A4	803	CLA	C2C-C1C-NC	3.15	113.35	110.09
14	B3	1815	CLA	C2C-C1C-NC	3.15	113.35	110.09
14	A1	809	CLA	C2C-C1C-NC	3.15	113.35	110.09
14	A5	807	CLA	C2C-C1C-NC	3.15	113.35	110.09
16	J4	103	BCR	C36-C18-C19	3.15	123.12	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A5	801	CLA	O2A-CGA-CBA	3.15	121.03	111.92
16	A4	849	BCR	C29-C30-C25	3.15	115.41	110.48
14	B1	815	CLA	C2C-C1C-NC	3.15	113.35	110.09
16	B4	846	BCR	C2-C1-C6	3.15	115.41	110.48
16	A2	1647	BCR	C29-C30-C25	3.15	115.41	110.48
14	B1	837	CLA	C2C-C1C-NC	3.15	113.36	110.09
14	B1	807	CLA	O2A-CGA-CBA	3.15	121.04	111.92
14	B5	1812	CLA	O2A-CGA-CBA	3.15	121.04	111.92
16	A1	843	BCR	C40-C30-C25	3.15	115.42	110.31
14	A2	1611	CLA	C2C-C1C-NC	3.16	113.36	110.09
14	B4	821	CLA	C2C-C1C-NC	3.16	113.36	110.09
14	A6	1610	CLA	C2C-C1C-NC	3.16	113.36	110.09
14	A3	838	CLA	C2C-C1C-NC	3.16	113.36	110.09
16	B6	844	BCR	C2-C1-C6	3.16	115.42	110.48
14	A5	813	CLA	O2A-CGA-CBA	3.16	121.05	111.92
14	B2	825	CLA	O2A-CGA-CBA	3.16	121.05	111.92
14	A5	837	CLA	O2D-CGD-CBD	3.16	116.88	111.28
14	A4	809	CLA	C2C-C1C-NC	3.16	113.36	110.09
14	B1	827	CLA	O2A-CGA-CBA	3.16	121.06	111.92
16	A3	850	BCR	C29-C30-C25	3.16	115.42	110.48
14	B3	1809	CLA	O2A-CGA-CBA	3.16	121.06	111.92
14	A2	1606	CLA	C2C-C1C-NC	3.16	113.36	110.09
14	B3	1807	CLA	O2A-CGA-CBA	3.16	121.06	111.92
16	A5	847	BCR	C2-C1-C6	3.16	115.42	110.48
16	A4	849	BCR	C32-C1-C6	3.16	115.44	110.31
16	B1	848	BCR	C29-C30-C25	3.16	115.42	110.48
14	B5	1829	CLA	CBA-CAA-C2A	3.16	123.20	113.82
14	A3	826	CLA	C2C-C1C-NC	3.16	113.37	110.09
14	A1	801	CLA	O2A-CGA-CBA	3.16	121.07	111.92
14	A3	825	CLA	O2A-CGA-CBA	3.16	121.07	111.92
14	A4	837	CLA	C2C-C1C-NC	3.16	113.37	110.09
14	B3	1816	CLA	C2C-C1C-NC	3.16	113.37	110.09
14	A4	824	CLA	O2A-CGA-CBA	3.17	121.07	111.92
16	B6	850	BCR	C29-C30-C25	3.17	115.43	110.48
14	B3	1829	CLA	C3C-C4C-NC	3.17	114.35	110.43
16	A1	842	BCR	C33-C5-C6	3.17	128.05	124.51
16	A2	1652	BCR	C29-C30-C25	3.17	115.43	110.48
16	A4	847	BCR	C2-C1-C6	3.17	115.43	110.48
14	A6	1637	CLA	C2C-C1C-NC	3.17	113.37	110.09
14	A5	838	CLA	C2C-C1C-NC	3.17	113.37	110.09
14	A1	812	CLA	O2A-CGA-CBA	3.17	121.09	111.92
14	B6	819	CLA	O2D-CGD-CBD	3.17	116.91	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1604	CLA	O2A-CGA-CBA	3.17	121.09	111.92
14	B4	809	CLA	O2A-CGA-CBA	3.17	121.09	111.92
14	A6	1611	CLA	C2C-C1C-NC	3.17	113.38	110.09
14	B1	854	CLA	O2D-CGD-CBD	3.17	116.91	111.28
17	A1	848	LHG	O8-C23-C24	3.17	121.10	111.92
14	B4	812	CLA	O2D-CGD-CBD	3.17	116.91	111.28
14	B3	1804	CLA	C3C-C4C-NC	3.18	114.36	110.43
14	A3	828	CLA	O2A-CGA-CBA	3.18	121.10	111.92
14	A5	810	CLA	C2C-C1C-NC	3.18	113.38	110.09
16	B2	842	BCR	C33-C5-C6	3.18	128.06	124.51
16	A3	851	BCR	C29-C30-C25	3.18	115.45	110.48
14	A3	834	CLA	C2C-C1C-NC	3.18	113.38	110.09
16	J5	104	BCR	C29-C30-C25	3.18	115.45	110.48
14	A6	1633	CLA	C2C-C1C-NC	3.18	113.38	110.09
14	B6	806	CLA	O2A-CGA-CBA	3.18	121.11	111.92
16	A1	842	BCR	C2-C1-C6	3.18	115.45	110.48
14	B5	1802	CLA	C2C-C1C-NC	3.18	113.38	110.09
16	A5	848	BCR	C2-C1-C6	3.18	115.45	110.48
14	A1	803	CLA	C2C-C1C-NC	3.18	113.38	110.09
16	F1	1302	BCR	C2-C1-C6	3.18	115.45	110.48
16	B2	843	BCR	C32-C1-C6	3.18	115.47	110.31
14	B4	837	CLA	C2C-C1C-NC	3.18	113.39	110.09
16	A3	847	BCR	C33-C5-C6	3.18	128.07	124.51
16	B3	1847	BCR	C33-C5-C6	3.19	128.07	124.51
14	B1	825	CLA	O2A-CGA-CBA	3.19	121.13	111.92
14	B1	854	CLA	O2A-CGA-CBA	3.19	121.13	111.92
17	A4	850	LHG	O7-C7-C8	3.19	118.27	111.55
14	A6	1628	CLA	O2A-CGA-CBA	3.19	121.15	111.92
14	B3	1815	CLA	O2A-CGA-CBA	3.19	121.15	111.92
16	F1	1302	BCR	C29-C30-C25	3.19	115.47	110.48
14	B4	829	CLA	CBA-CAA-C2A	3.19	123.29	113.82
14	B4	811	CLA	O2A-CGA-CBA	3.19	121.15	111.92
14	A3	829	CLA	CMB-C2B-C3B	3.19	130.69	124.88
14	L1	207	CLA	C2C-C1C-NC	3.19	113.40	110.09
17	A6	1649	LHG	O7-C7-C8	3.19	118.28	111.55
14	A2	1636	CLA	O2D-CGD-CBD	3.19	116.95	111.28
14	B6	803	CLA	O2A-CGA-CBA	3.19	121.16	111.92
17	A5	851	LHG	O7-C7-C8	3.20	118.29	111.55
14	B5	1838	CLA	C2C-C1C-NC	3.20	113.40	110.09
14	B4	804	CLA	O2A-CGA-CBA	3.20	121.16	111.92
14	B3	1840	CLA	O2A-CGA-CBA	3.20	121.16	111.92
14	B2	806	CLA	O2A-CGA-CBA	3.20	121.16	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	813	CLA	O2A-CGA-CBA	3.20	121.16	111.92
14	A4	842	CLA	C2C-C1C-NC	3.20	113.40	110.09
14	L5	206	CLA	C2C-C1C-NC	3.20	113.40	110.09
14	B2	804	CLA	O2A-CGA-CBA	3.20	121.17	111.92
14	B3	1818	CLA	O2A-CGA-CBA	3.20	121.17	111.92
14	B6	839	CLA	O2A-CGA-CBA	3.20	121.17	111.92
14	A2	1615	CLA	O2A-CGA-CBA	3.20	121.17	111.92
14	B1	828	CLA	C3C-C4C-NC	3.20	114.39	110.43
14	A6	1626	CLA	C2C-C1C-NC	3.20	113.41	110.09
14	B1	809	CLA	O2A-CGA-CBA	3.20	121.18	111.92
14	B2	838	CLA	C2C-C1C-NC	3.20	113.41	110.09
14	B5	1818	CLA	O2A-CGA-CBA	3.20	121.19	111.92
14	A1	828	CLA	CMB-C2B-C3B	3.20	130.72	124.88
14	A6	1629	CLA	CMB-C2B-C3B	3.20	130.72	124.88
14	A2	1612	CLA	C2C-C1C-NC	3.21	113.41	110.09
14	B5	1829	CLA	C2C-C1C-NC	3.21	113.41	110.09
14	B4	808	CLA	O2D-CGD-CBD	3.21	116.97	111.28
14	A3	812	CLA	O2A-CGA-CBA	3.21	121.19	111.92
14	B5	1828	CLA	O2A-CGA-CBA	3.21	121.19	111.92
14	B2	812	CLA	O2A-CGA-CBA	3.21	121.19	111.92
16	B6	847	BCR	C33-C5-C6	3.21	128.10	124.51
14	A2	1613	CLA	C2C-C1C-NC	3.21	113.41	110.09
14	B6	814	CLA	C2C-C1C-NC	3.21	113.41	110.09
14	B6	816	CLA	O2A-CGA-CBA	3.21	121.20	111.92
17	A2	1653	LHG	O7-C7-C8	3.21	118.32	111.55
14	B3	1828	CLA	O2A-CGA-CBA	3.21	121.20	111.92
14	B5	1816	CLA	C2C-C1C-NC	3.21	113.42	110.09
14	A2	1621	CLA	O2D-CGD-CBD	3.21	116.98	111.28
16	F4	203	BCR	C29-C30-C25	3.21	115.50	110.48
16	B3	1849	BCR	C33-C5-C6	3.21	128.10	124.51
14	B4	840	CLA	O2A-CGA-CBA	3.21	121.21	111.92
14	M2	1201	CLA	O2A-CGA-CBA	3.21	121.21	111.92
14	B6	813	CLA	C2C-C1C-NC	3.21	113.42	110.09
14	A3	813	CLA	C2C-C1C-NC	3.21	113.42	110.09
14	B4	818	CLA	O2A-CGA-CBA	3.21	121.22	111.92
14	A4	825	CLA	C2C-C1C-NC	3.22	113.42	110.09
14	L2	202	CLA	C2C-C1C-NC	3.22	113.42	110.09
14	L5	203	CLA	C2C-C1C-NC	3.22	113.42	110.09
14	B2	837	CLA	O2A-CGA-CBA	3.22	121.23	111.92
14	B1	839	CLA	O2A-CGA-CBA	3.22	121.23	111.92
16	B3	1846	BCR	C2-C1-C6	3.22	115.51	110.48
14	B2	816	CLA	O2D-CGD-CBD	3.22	116.99	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	810	CLA	O2D-CGD-CBD	3.22	116.99	111.28
16	F2	203	BCR	C29-C30-C25	3.22	115.52	110.48
16	A1	842	BCR	C29-C30-C25	3.22	115.52	110.48
14	B4	813	CLA	O2D-CGD-CBD	3.22	117.00	111.28
14	A5	829	CLA	CMB-C2B-C3B	3.23	130.75	124.88
14	A4	805	CLA	C2C-C1C-NC	3.23	113.43	110.09
14	L1	202	CLA	C2C-C1C-NC	3.23	113.43	110.09
14	A1	839	CLA	O2D-CGD-CBD	3.23	117.00	111.28
16	F5	1302	BCR	C29-C30-C25	3.23	115.52	110.48
16	F5	1302	BCR	C2-C1-C6	3.23	115.53	110.48
14	B2	812	CLA	C2C-C1C-NC	3.23	113.43	110.09
14	B1	814	CLA	O2A-CGA-CBA	3.23	121.26	111.92
14	A6	1651	CLA	O2A-CGA-CBA	3.23	121.26	111.92
14	M6	1201	CLA	O2A-CGA-CBA	3.23	121.26	111.92
16	B4	846	BCR	C32-C1-C6	3.23	115.55	110.31
14	A3	801	CLA	O2A-CGA-CBA	3.23	121.26	111.92
17	A5	851	LHG	O8-C23-C24	3.23	121.26	111.92
16	B5	1846	BCR	C2-C1-C6	3.23	115.53	110.48
14	A2	1631	CLA	CMB-C2B-C3B	3.23	130.76	124.88
16	F3	203	BCR	C2-C1-C6	3.23	115.53	110.48
14	B1	817	CLA	O2A-CGA-CBA	3.23	121.27	111.92
16	J2	102	BCR	C2-C1-C6	3.23	115.53	110.48
14	A4	828	CLA	CMB-C2B-C3B	3.23	130.77	124.88
14	J6	1101	CLA	O2A-CGA-CBA	3.24	121.28	111.92
14	A6	1612	CLA	O2A-CGA-CBA	3.24	121.28	111.92
14	B2	826	CLA	CBA-CAA-C2A	3.24	123.42	113.82
16	A6	1646	BCR	C2-C1-C6	3.24	115.54	110.48
14	B6	810	CLA	O2A-CGA-CBA	3.24	121.28	111.92
14	B3	1812	CLA	O2A-CGA-CBA	3.24	121.28	111.92
14	A4	838	CLA	O2A-CGA-CBA	3.24	121.29	111.92
14	A3	828	CLA	C2C-C1C-NC	3.24	113.44	110.09
16	B1	849	BCR	C2-C1-C6	3.24	115.55	110.48
14	B6	827	CLA	C3C-C4C-NC	3.24	114.44	110.43
14	A4	811	CLA	O2A-CGA-CBA	3.24	121.30	111.92
16	F4	201	BCR	C29-C30-C25	3.24	115.55	110.48
14	A2	1602	CLA	O2A-CGA-CBA	3.24	121.30	111.92
14	A1	807	CLA	O2A-CGA-CBA	3.24	121.30	111.92
14	A3	810	CLA	O2D-CGD-CBD	3.24	117.03	111.28
14	B6	838	CLA	O2A-CGA-CBA	3.24	121.30	111.92
14	B4	806	CLA	C2C-C1C-NC	3.25	113.45	110.09
14	A1	832	CLA	O2D-CGD-CBD	3.25	117.04	111.28
14	A4	818	CLA	C2C-C1C-NC	3.25	113.45	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B5	1846	BCR	C32-C1-C6	3.25	115.57	110.31
14	B2	809	CLA	O2D-CGD-CBD	3.25	117.04	111.28
14	B3	1821	CLA	O2D-CGD-CBD	3.25	117.04	111.28
14	A3	832	CLA	C2C-C1C-NC	3.25	113.45	110.09
14	A5	832	CLA	C2C-C1C-NC	3.25	113.46	110.09
16	A3	847	BCR	C38-C26-C25	3.25	128.15	124.51
14	B3	1804	CLA	O2A-CGA-CBA	3.25	121.33	111.92
14	A3	838	CLA	O2D-CGD-CBD	3.25	117.05	111.28
17	A2	1654	LHG	O7-C7-C8	3.25	118.41	111.55
14	B3	1827	CLA	C2C-C1C-NC	3.25	113.46	110.09
14	A3	840	CLA	O2A-CGA-CBA	3.25	121.33	111.92
16	A5	848	BCR	C40-C30-C25	3.25	115.58	110.31
14	A6	1628	CLA	O2D-CGD-CBD	3.25	117.05	111.28
14	A2	1608	CLA	C2C-C1C-NC	3.26	113.46	110.09
14	B5	1819	CLA	O2D-CGD-CBD	3.26	117.06	111.28
14	L4	201	CLA	C2C-C1C-NC	3.26	113.46	110.09
14	B1	808	CLA	C2C-C1C-NC	3.26	113.46	110.09
16	A3	847	BCR	C2-C1-C6	3.26	115.57	110.48
14	A4	833	CLA	O2D-CGD-CBD	3.26	117.06	111.28
14	A4	807	CLA	O2A-CGA-CBA	3.26	121.34	111.92
14	B3	1829	CLA	CBA-CAA-C2A	3.26	123.49	113.82
16	A6	1645	BCR	C2-C1-C6	3.26	115.58	110.48
14	B4	815	CLA	O2A-CGA-CBA	3.26	121.35	111.92
14	A6	1623	CLA	C2C-C1C-NC	3.26	113.47	110.09
14	B3	1812	CLA	O2D-CGD-CBD	3.26	117.06	111.28
16	J6	1105	BCR	C29-C30-C25	3.26	115.58	110.48
14	A4	810	CLA	C2C-C1C-NC	3.26	113.47	110.09
14	A5	808	CLA	O2A-CGA-CBA	3.26	121.35	111.92
14	A3	839	CLA	C2C-C1C-NC	3.26	113.47	110.09
14	B4	812	CLA	O2A-CGA-CBA	3.27	121.36	111.92
16	A5	845	BCR	C2-C1-C6	3.27	115.58	110.48
16	A4	847	BCR	C40-C30-C25	3.27	115.61	110.31
16	B6	843	BCR	C33-C5-C6	3.27	128.17	124.51
14	A5	812	CLA	O2A-CGA-CBA	3.27	121.37	111.92
14	B5	1840	CLA	O2A-CGA-CBA	3.27	121.37	111.92
17	A3	853	LHG	O7-C7-C8	3.27	118.44	111.55
14	A2	1621	CLA	C2C-C1C-NC	3.27	113.47	110.09
14	B2	824	CLA	C2C-C1C-NC	3.27	113.48	110.09
14	A1	810	CLA	C2C-C1C-NC	3.27	113.48	110.09
14	B1	828	CLA	C2C-C1C-NC	3.27	113.48	110.09
16	A6	1643	BCR	C38-C26-C25	3.27	128.17	124.51
16	B1	844	BCR	C32-C1-C6	3.27	115.61	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	812	CLA	O2D-CGD-CBD	3.27	117.08	111.28
17	A5	852	LHG	O7-C7-C8	3.27	118.45	111.55
16	A6	1643	BCR	C2-C1-C6	3.27	115.60	110.48
14	A5	842	CLA	O2D-CGD-CBD	3.27	117.09	111.28
14	A3	819	CLA	O2D-CGD-CBD	3.28	117.09	111.28
14	A5	804	CLA	C2C-C1C-NC	3.28	113.48	110.09
17	A4	851	LHG	O7-C7-C8	3.28	118.46	111.55
14	A5	811	CLA	C2C-C1C-NC	3.28	113.48	110.09
14	A5	834	CLA	O2D-CGD-CBD	3.28	117.09	111.28
16	F2	203	BCR	C2-C1-C6	3.28	115.60	110.48
14	A3	811	CLA	C2C-C1C-NC	3.28	113.48	110.09
14	A5	828	CLA	C2C-C1C-NC	3.28	113.48	110.09
16	J1	104	BCR	C29-C30-C25	3.28	115.60	110.48
14	B1	828	CLA	CBA-CAA-C2A	3.28	123.55	113.82
16	J4	103	BCR	C38-C26-C25	3.28	128.18	124.51
16	A2	1650	BCR	C2-C1-C6	3.28	115.61	110.48
16	B1	844	BCR	C2-C1-C6	3.28	115.61	110.48
14	B5	1829	CLA	C3C-C4C-NC	3.28	114.49	110.43
14	A3	803	CLA	O2A-CGA-CBA	3.28	121.41	111.92
16	A6	1643	BCR	C33-C5-C6	3.28	128.18	124.51
14	B5	1808	CLA	C2C-C1C-NC	3.28	113.49	110.09
16	B5	1849	BCR	C33-C5-C6	3.28	128.18	124.51
14	A1	818	CLA	CMB-C2B-C3B	3.28	130.86	124.88
16	A3	856	BCR	C2-C1-C6	3.28	115.61	110.48
14	M2	1201	CLA	C2C-C1C-NC	3.29	113.49	110.09
14	B4	802	CLA	C2C-C1C-NC	3.29	113.49	110.09
14	B3	1843	CLA	C2C-C1C-NC	3.29	113.49	110.09
14	B5	1809	CLA	O2A-CGA-CBA	3.29	121.43	111.92
14	A3	843	CLA	O2D-CGD-CBD	3.29	117.11	111.28
14	A3	828	CLA	O2D-CGD-CBD	3.29	117.11	111.28
16	A3	850	BCR	C40-C30-C25	3.29	115.64	110.31
14	B4	838	CLA	C2C-C1C-NC	3.29	113.50	110.09
16	B3	1849	BCR	C2-C1-C6	3.29	115.62	110.48
16	B5	1847	BCR	C2-C1-C6	3.29	115.62	110.48
14	A2	1605	CLA	O2A-CGA-CBA	3.29	121.44	111.92
14	A1	805	CLA	C2C-C1C-NC	3.29	113.50	110.09
16	A2	1652	BCR	C32-C1-C6	3.29	115.65	110.31
14	B1	841	CLA	C2C-C1C-NC	3.30	113.50	110.09
14	B4	843	CLA	C2C-C1C-NC	3.30	113.50	110.09
16	A1	844	BCR	C2-C1-C6	3.30	115.63	110.48
16	A4	844	BCR	C2-C1-C6	3.30	115.63	110.48
14	B3	1808	CLA	C2C-C1C-NC	3.30	113.50	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B1	802	CLA	C2C-C1C-NC	3.30	113.51	110.09
14	A5	839	CLA	O2A-CGA-CBA	3.30	121.46	111.92
14	B6	825	CLA	C2C-C1C-NC	3.30	113.51	110.09
14	A3	819	CLA	CMB-C2B-C3B	3.30	130.89	124.88
16	F2	201	BCR	C29-C30-C25	3.30	115.64	110.48
16	B1	843	BCR	C33-C5-C6	3.31	128.21	124.51
16	J6	1104	BCR	C38-C26-C25	3.31	128.21	124.51
16	F3	201	BCR	C29-C30-C25	3.31	115.65	110.48
14	B5	1827	CLA	C2C-C1C-NC	3.31	113.51	110.09
16	B6	844	BCR	C32-C1-C6	3.31	115.67	110.31
16	J5	103	BCR	C38-C26-C25	3.31	128.21	124.51
17	A6	1650	LHG	O7-C7-C8	3.31	118.53	111.55
16	M6	1202	BCR	C1-C6-C7	3.31	125.03	115.73
16	A3	850	BCR	C2-C1-C6	3.31	115.66	110.48
14	L6	203	CLA	O2A-CGA-CBA	3.31	121.50	111.92
16	B4	849	BCR	C2-C1-C6	3.31	115.66	110.48
16	M4	101	BCR	C1-C6-C7	3.31	125.04	115.73
14	A6	1603	CLA	C2C-C1C-NC	3.31	113.52	110.09
14	A2	1630	CLA	O2D-CGD-CBD	3.31	117.16	111.28
14	B2	809	CLA	O2A-CGA-CBA	3.32	121.51	111.92
14	L3	205	CLA	C2C-C1C-NC	3.32	113.52	110.09
14	I6	101	CLA	O2A-CGA-CBA	3.32	121.51	111.92
16	M2	1202	BCR	C1-C6-C7	3.32	125.05	115.73
16	J2	103	BCR	C29-C30-C25	3.32	115.66	110.48
14	B6	806	CLA	C2C-C1C-NC	3.32	113.52	110.09
14	B2	818	CLA	O2D-CGD-CBD	3.32	117.17	111.28
16	A5	853	BCR	C2-C1-C6	3.32	115.67	110.48
14	B6	839	CLA	C2C-C1C-NC	3.32	113.53	110.09
14	B5	1841	CLA	C2C-C1C-NC	3.32	113.53	110.09
14	B4	827	CLA	C2C-C1C-NC	3.32	113.53	110.09
14	B2	806	CLA	C2C-C1C-NC	3.32	113.53	110.09
16	J1	103	BCR	C2-C1-C6	3.32	115.67	110.48
16	J3	104	BCR	C29-C30-C25	3.32	115.67	110.48
16	F4	203	BCR	C2-C1-C6	3.32	115.67	110.48
14	B6	827	CLA	CBA-CAA-C2A	3.32	123.68	113.82
16	B1	845	BCR	C2-C1-C6	3.33	115.68	110.48
16	B1	845	BCR	C33-C5-C6	3.33	128.23	124.51
16	A2	1647	BCR	C2-C1-C6	3.33	115.68	110.48
16	A6	1643	BCR	C29-C30-C25	3.33	115.68	110.48
14	A6	1619	CLA	CMB-C2B-C3B	3.33	130.94	124.88
16	J6	1104	BCR	C2-C1-C6	3.33	115.69	110.48
16	B4	850	BCR	C2-C1-C6	3.33	115.69	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A2	1647	BCR	C38-C26-C25	3.33	128.24	124.51
14	A2	1610	CLA	O2A-CGA-CBA	3.33	121.55	111.92
14	A1	811	CLA	O2A-CGA-CBA	3.33	121.56	111.92
14	B3	1831	CLA	CMB-C2B-C3B	3.34	130.95	124.88
16	B4	849	BCR	C33-C5-C6	3.34	128.24	124.51
14	B5	1801	CLA	O2A-CGA-CBA	3.34	121.57	111.92
14	B6	829	CLA	CMB-C2B-C3B	3.34	130.96	124.88
14	L1	201	CLA	C2C-C1C-NC	3.34	113.55	110.09
14	B5	1809	CLA	C2C-C1C-NC	3.34	113.55	110.09
14	B6	811	CLA	O2D-CGD-CBD	3.34	117.20	111.28
16	J4	104	BCR	C29-C30-C25	3.34	115.70	110.48
16	A3	852	BCR	C32-C1-C6	3.34	115.72	110.31
16	L3	201	BCR	C2-C1-C6	3.34	115.70	110.48
14	B3	1802	CLA	C2C-C1C-NC	3.34	113.55	110.09
16	M3	1602	BCR	C1-C6-C7	3.34	125.11	115.73
14	A2	1626	CLA	O2D-CGD-CBD	3.34	117.20	111.28
14	B5	1821	CLA	C2C-C1C-NC	3.34	113.55	110.09
14	A6	1634	CLA	O2D-CGD-CBD	3.34	117.21	111.28
14	B1	807	CLA	C2C-C1C-NC	3.34	113.55	110.09
16	F6	203	BCR	C2-C1-C6	3.34	115.71	110.48
16	B4	847	BCR	C33-C5-C6	3.34	128.25	124.51
14	A6	1628	CLA	C2C-C1C-NC	3.35	113.55	110.09
16	B2	846	BCR	C2-C1-C6	3.35	115.71	110.48
14	A6	1638	CLA	C2C-C1C-NC	3.35	113.56	110.09
14	A3	819	CLA	C2C-C1C-NC	3.35	113.56	110.09
16	B6	847	BCR	C2-C1-C6	3.35	115.71	110.48
14	B5	1804	CLA	O2A-CGA-CBA	3.35	121.60	111.92
16	B2	846	BCR	C33-C5-C6	3.35	128.26	124.51
14	A2	1641	CLA	O2A-CGA-CBA	3.35	121.61	111.92
14	A4	815	CLA	C2C-C1C-NC	3.36	113.56	110.09
14	A1	802	CLA	O2A-CGA-CBA	3.36	121.62	111.92
14	A4	826	CLA	O2A-CGA-CBA	3.36	121.62	111.92
14	A1	809	CLA	O2D-CGD-CBD	3.36	117.23	111.28
16	B5	1850	BCR	C29-C30-C25	3.36	115.73	110.48
14	L2	207	CLA	C2C-C1C-NC	3.36	113.57	110.09
16	J4	103	BCR	C2-C1-C6	3.36	115.73	110.48
16	B4	846	BCR	C29-C30-C25	3.36	115.73	110.48
14	A5	807	CLA	O2A-CGA-CBA	3.36	121.64	111.92
16	B4	847	BCR	C2-C1-C6	3.36	115.73	110.48
14	B2	826	CLA	C3C-C4C-NC	3.36	114.59	110.43
16	A1	845	BCR	C40-C30-C25	3.36	115.76	110.31
14	A1	818	CLA	C2C-C1C-NC	3.36	113.57	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M1	1202	BCR	C1-C6-C7	3.37	125.19	115.73
14	A3	843	CLA	O2A-CGA-CBA	3.37	121.66	111.92
14	B2	815	CLA	O2A-CGA-CBA	3.37	121.66	111.92
14	B2	840	CLA	C2C-C1C-NC	3.37	113.58	110.09
14	A1	815	CLA	C2C-C1C-NC	3.37	113.58	110.09
17	A3	854	LHG	O7-C7-C8	3.37	118.66	111.55
16	A1	842	BCR	C38-C26-C25	3.37	128.28	124.51
16	B5	1846	BCR	C29-C30-C25	3.37	115.75	110.48
16	A5	850	BCR	C32-C1-C6	3.37	115.78	110.31
14	B2	802	CLA	O2A-CGA-CBA	3.37	121.68	111.92
14	A3	835	CLA	O2D-CGD-CBD	3.38	117.27	111.28
14	A2	1614	CLA	O2A-CGA-CBA	3.38	121.68	111.92
16	A1	847	BCR	C32-C1-C6	3.38	115.78	110.31
14	A6	1608	CLA	O2A-CGA-CBA	3.38	121.69	111.92
14	A1	827	CLA	C2C-C1C-NC	3.38	113.59	110.09
16	A6	1652	BCR	C2-C1-C6	3.38	115.76	110.48
16	B1	847	BCR	C33-C5-C6	3.38	128.29	124.51
14	B4	824	CLA	O2D-CGD-CBD	3.38	117.28	111.28
16	A3	847	BCR	C29-C30-C25	3.38	115.77	110.48
16	F6	201	BCR	C33-C5-C6	3.38	128.29	124.51
14	B1	830	CLA	C2C-C1C-NC	3.38	113.59	110.09
14	A3	837	CLA	O2D-CGD-CBD	3.38	117.28	111.28
16	B1	847	BCR	C2-C1-C6	3.38	115.77	110.48
14	A5	816	CLA	C2C-C1C-NC	3.39	113.59	110.09
16	J5	103	BCR	C2-C1-C6	3.39	115.77	110.48
14	A5	817	CLA	O2D-CGD-CBD	3.39	117.28	111.28
14	A2	1602	CLA	C2C-C1C-NC	3.39	113.60	110.09
16	J3	103	BCR	C2-C1-C6	3.39	115.77	110.48
16	B6	844	BCR	C29-C30-C25	3.39	115.77	110.48
14	L6	202	CLA	C2C-C1C-NC	3.39	113.60	110.09
14	B4	806	CLA	O2A-CGA-CBA	3.39	121.72	111.92
16	A6	1646	BCR	C40-C30-C25	3.39	115.80	110.31
14	B6	807	CLA	C2C-C1C-NC	3.39	113.60	110.09
14	A4	802	CLA	O2A-CGA-CBA	3.39	121.72	111.92
14	B1	840	CLA	C2C-C1C-NC	3.39	113.60	110.09
14	A4	831	CLA	C2C-C1C-NC	3.39	113.60	110.09
16	B5	1849	BCR	C2-C1-C6	3.39	115.78	110.48
14	B1	826	CLA	C2C-C1C-NC	3.39	113.60	110.09
14	A3	827	CLA	O2A-CGA-CBA	3.39	121.73	111.92
16	B5	1847	BCR	C33-C5-C6	3.39	128.31	124.51
16	A5	845	BCR	C29-C30-C25	3.39	115.78	110.48
14	A2	1634	CLA	C2C-C1C-NC	3.40	113.61	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A2	1625	CLA	C2C-C1C-NC	3.40	113.61	110.09
16	A2	1650	BCR	C40-C30-C25	3.40	115.82	110.31
14	B5	1831	CLA	CMB-C2B-C3B	3.40	131.07	124.88
14	A3	817	CLA	O2D-CGD-CBD	3.40	117.31	111.28
14	B3	1831	CLA	C2C-C1C-NC	3.40	113.61	110.09
14	B5	1806	CLA	O2A-CGA-CBA	3.40	121.75	111.92
16	B1	844	BCR	C29-C30-C25	3.40	115.80	110.48
14	B1	809	CLA	C2C-C1C-NC	3.40	113.61	110.09
14	A1	822	CLA	C2C-C1C-NC	3.40	113.61	110.09
16	B6	850	BCR	C33-C5-C6	3.41	128.32	124.51
14	A5	819	CLA	C2C-C1C-NC	3.41	113.62	110.09
16	J3	103	BCR	C38-C26-C25	3.41	128.32	124.51
14	B5	1824	CLA	O2D-CGD-CBD	3.41	117.33	111.28
16	L6	201	BCR	C2-C1-C6	3.41	115.81	110.48
14	A2	1612	CLA	O2D-CGD-CBD	3.41	117.33	111.28
16	M5	101	BCR	C1-C6-C7	3.41	125.31	115.73
16	L5	201	BCR	C2-C1-C6	3.41	115.81	110.48
14	B3	1824	CLA	O2D-CGD-CBD	3.41	117.33	111.28
14	B4	841	CLA	C2C-C1C-NC	3.41	113.62	110.09
14	B6	841	CLA	C2C-C1C-NC	3.41	113.62	110.09
14	A2	1604	CLA	C2C-C1C-NC	3.41	113.62	110.09
14	I6	101	CLA	C2C-C1C-NC	3.41	113.62	110.09
14	B5	1831	CLA	C2C-C1C-NC	3.41	113.62	110.09
16	B6	845	BCR	C2-C1-C6	3.41	115.82	110.48
16	B5	1850	BCR	C2-C1-C6	3.42	115.82	110.48
14	B2	805	CLA	C2C-C1C-NC	3.42	113.63	110.09
14	A2	1618	CLA	C2C-C1C-NC	3.42	113.63	110.09
14	B1	823	CLA	O2D-CGD-CBD	3.42	117.34	111.28
14	A6	1636	CLA	O2D-CGD-CBD	3.42	117.35	111.28
14	A4	822	CLA	C2C-C1C-NC	3.42	113.63	110.09
14	B1	803	CLA	O2A-CGA-CBA	3.42	121.81	111.92
14	L6	208	CLA	C2C-C1C-NC	3.42	113.63	110.09
14	B5	1843	CLA	C2C-C1C-NC	3.42	113.64	110.09
14	B4	809	CLA	C2C-C1C-NC	3.42	113.64	110.09
16	F2	201	BCR	C2-C1-C6	3.43	115.83	110.48
14	B3	1813	CLA	O2D-CGD-CBD	3.43	117.36	111.28
14	A3	823	CLA	C2C-C1C-NC	3.43	113.64	110.09
16	J4	104	BCR	C2-C1-C6	3.43	115.84	110.48
14	A2	1631	CLA	O2A-CGA-CBA	3.43	121.85	111.92
16	B2	847	BCR	C2-C1-C6	3.43	115.85	110.48
14	A4	823	CLA	O2D-CGD-CBD	3.43	117.37	111.28
14	A5	803	CLA	O2A-CGA-CBA	3.43	121.85	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B3	1846	BCR	C32-C1-C6	3.43	115.88	110.31
14	A4	827	CLA	C2C-C1C-NC	3.44	113.65	110.09
16	F3	201	BCR	C33-C5-C6	3.44	128.35	124.51
14	A4	818	CLA	O2D-CGD-CBD	3.44	117.38	111.28
14	B1	818	CLA	O2D-CGD-CBD	3.44	117.38	111.28
16	B2	844	BCR	C33-C5-C6	3.44	128.36	124.51
14	A1	823	CLA	O2D-CGD-CBD	3.44	117.38	111.28
16	B2	843	BCR	C29-C30-C25	3.44	115.86	110.48
14	A1	812	CLA	O2D-CGD-CBD	3.44	117.38	111.28
14	B3	1807	CLA	C2C-C1C-NC	3.44	113.65	110.09
14	A1	826	CLA	O2A-CGA-CBA	3.44	121.87	111.92
14	A3	824	CLA	O2D-CGD-CBD	3.44	117.39	111.28
14	B1	818	CLA	O2A-CGA-CBA	3.44	121.88	111.92
16	A1	847	BCR	C2-C1-C6	3.44	115.86	110.48
14	B2	804	CLA	C2C-C1C-NC	3.44	113.66	110.09
14	A1	819	CLA	O2A-CGA-CBA	3.45	121.88	111.92
14	A4	818	CLA	CMB-C2B-C3B	3.45	131.15	124.88
14	A4	827	CLA	O2D-CGD-CBD	3.45	117.39	111.28
14	B3	1841	CLA	C2C-C1C-NC	3.45	113.66	110.09
14	A5	810	CLA	O2D-CGD-CBD	3.45	117.39	111.28
14	A5	819	CLA	O2D-CGD-CBD	3.45	117.39	111.28
14	A4	809	CLA	O2D-CGD-CBD	3.45	117.40	111.28
14	B4	821	CLA	O2D-CGD-CBD	3.45	117.40	111.28
14	B1	805	CLA	O2A-CGA-CBA	3.45	121.90	111.92
14	B2	816	CLA	O2A-CGA-CBA	3.45	121.90	111.92
14	B2	810	CLA	O2D-CGD-CBD	3.45	117.40	111.28
14	A4	841	CLA	O2A-CGA-CBA	3.45	121.90	111.92
14	A1	806	CLA	O2A-CGA-CBA	3.45	121.91	111.92
14	A1	834	CLA	O2D-CGD-CBD	3.45	117.41	111.28
16	B2	850	BCR	C33-C5-C6	3.45	128.37	124.51
14	A5	819	CLA	CMB-C2B-C3B	3.45	131.17	124.88
14	A2	1620	CLA	O2D-CGD-CBD	3.45	117.41	111.28
14	A5	842	CLA	O2A-CGA-CBA	3.46	121.91	111.92
14	B5	1821	CLA	O2D-CGD-CBD	3.46	117.41	111.28
14	B1	830	CLA	CMB-C2B-C3B	3.46	131.18	124.88
14	A6	1617	CLA	O2D-CGD-CBD	3.46	117.41	111.28
14	A3	816	CLA	C2C-C1C-NC	3.46	113.67	110.09
16	L2	201	BCR	C2-C1-C6	3.46	115.89	110.48
14	A6	1618	CLA	O2D-CGD-CBD	3.46	117.42	111.28
14	A6	1624	CLA	O2D-CGD-CBD	3.46	117.42	111.28
16	J2	102	BCR	C38-C26-C25	3.47	128.39	124.51
14	A5	823	CLA	C2C-C1C-NC	3.47	113.68	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A4	851	LHG	O8-C23-C24	3.47	120.47	111.38
14	A2	1619	CLA	O2D-CGD-CBD	3.47	117.43	111.28
16	B5	1850	BCR	C33-C5-C6	3.47	128.39	124.51
14	B3	1809	CLA	C2C-C1C-NC	3.47	113.68	110.09
14	A3	807	CLA	O2D-CGD-CBD	3.47	117.44	111.28
14	A5	827	CLA	O2A-CGA-CBA	3.47	121.96	111.92
16	B2	844	BCR	C2-C1-C6	3.47	115.91	110.48
14	A4	822	CLA	O2A-CGA-CBA	3.47	121.97	111.92
16	A6	1648	BCR	C32-C1-C6	3.47	115.94	110.31
14	A4	817	CLA	O2D-CGD-CBD	3.48	117.44	111.28
14	B4	808	CLA	C2C-C1C-NC	3.48	113.69	110.09
16	F2	201	BCR	C33-C5-C6	3.48	128.40	124.51
16	B1	848	BCR	C2-C1-C6	3.48	115.92	110.48
14	A2	1625	CLA	O2A-CGA-CBA	3.48	121.98	111.92
14	A6	1616	CLA	C2C-C1C-NC	3.48	113.69	110.09
16	A2	1652	BCR	C2-C1-C6	3.48	115.92	110.48
14	B4	831	CLA	CMB-C2B-C3B	3.48	131.22	124.88
14	A6	1619	CLA	C2C-C1C-NC	3.48	113.70	110.09
16	A5	850	BCR	C2-C1-C6	3.48	115.93	110.48
16	A2	1648	BCR	C2-C1-C6	3.48	115.93	110.48
14	B5	1807	CLA	C2C-C1C-NC	3.49	113.70	110.09
16	A1	846	BCR	C38-C26-C25	3.49	128.41	124.51
16	A5	845	BCR	C38-C26-C25	3.49	128.41	124.51
14	A6	1619	CLA	O2D-CGD-CBD	3.49	117.47	111.28
14	A5	813	CLA	O2D-CGD-CBD	3.49	117.48	111.28
14	B4	819	CLA	O2D-CGD-CBD	3.49	117.48	111.28
14	F2	202	CLA	O2D-CGD-CBD	3.49	117.48	111.28
16	L5	201	BCR	C33-C5-C6	3.50	128.42	124.51
14	A3	808	CLA	O2A-CGA-CBA	3.50	122.03	111.92
14	B4	831	CLA	C2C-C1C-NC	3.50	113.71	110.09
14	A2	1629	CLA	O2A-CGA-CBA	3.50	122.03	111.92
17	X3	101	LHG	O7-C7-C8	3.50	118.93	111.55
14	A5	824	CLA	O2D-CGD-CBD	3.50	117.49	111.28
14	B2	828	CLA	CMB-C2B-C3B	3.50	131.26	124.88
14	A2	1621	CLA	CMB-C2B-C3B	3.50	131.26	124.88
16	J6	1105	BCR	C2-C1-C6	3.51	115.96	110.48
14	B6	808	CLA	C2C-C1C-NC	3.51	113.72	110.09
14	A2	1643	CLA	O2D-CGD-CBD	3.51	117.50	111.28
14	B6	818	CLA	CMB-C2B-C3B	3.51	131.27	124.88
17	A2	1654	LHG	O8-C23-C24	3.51	120.58	111.38
16	J1	104	BCR	C2-C1-C6	3.51	115.97	110.48
16	J5	104	BCR	C2-C1-C6	3.51	115.97	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A2	1644	CLA	O2A-CGA-CBA	3.51	122.08	111.92
14	B6	817	CLA	O2A-CGA-CBA	3.52	122.08	111.92
14	B3	1806	CLA	O2A-CGA-CBA	3.52	122.08	111.92
14	B2	807	CLA	C2C-C1C-NC	3.52	113.73	110.09
14	A2	1642	CLA	C2C-C1C-NC	3.52	113.73	110.09
14	A6	1607	CLA	O2D-CGD-CBD	3.52	117.52	111.28
16	A3	852	BCR	C2-C1-C6	3.52	115.98	110.48
14	L4	205	CLA	C2C-C1C-NC	3.52	113.73	110.09
16	J6	1104	BCR	C29-C30-C25	3.52	115.98	110.48
16	L1	209	BCR	C2-C1-C6	3.52	115.98	110.48
16	A5	849	BCR	C38-C26-C25	3.52	128.45	124.51
14	A6	1623	CLA	O2A-CGA-CBA	3.52	122.10	111.92
14	A3	823	CLA	O2A-CGA-CBA	3.52	122.11	111.92
16	J3	103	BCR	C29-C30-C25	3.53	115.99	110.48
14	A2	1630	CLA	C2C-C1C-NC	3.53	113.74	110.09
14	A4	808	CLA	O2D-CGD-CBD	3.53	117.53	111.28
16	A6	1644	BCR	C2-C1-C6	3.53	115.99	110.48
14	B1	824	CLA	O2D-CGD-CBD	3.53	117.53	111.28
14	A6	1610	CLA	O2D-CGD-CBD	3.53	117.54	111.28
14	A5	801	CLA	C2C-C1C-NC	3.53	113.74	110.09
14	B3	1820	CLA	CMB-C2B-C3B	3.53	131.31	124.88
14	A4	801	CLA	C2C-C1C-NC	3.53	113.75	110.09
16	B3	1846	BCR	C29-C30-C25	3.53	116.00	110.48
17	X4	101	LHG	O7-C7-C8	3.53	119.00	111.55
14	A2	1644	CLA	C2C-C1C-NC	3.53	113.75	110.09
16	B1	852	BCR	C33-C5-C6	3.54	128.47	124.51
17	B1	851	LHG	O7-C7-C8	3.54	119.01	111.55
14	A3	809	CLA	O2D-CGD-CBD	3.54	117.55	111.28
14	A3	826	CLA	O2D-CGD-CBD	3.54	117.55	111.28
16	B3	1847	BCR	C2-C1-C6	3.54	116.01	110.48
16	L6	209	BCR	C33-C5-C6	3.54	128.47	124.51
16	A5	846	BCR	C2-C1-C6	3.54	116.01	110.48
16	F4	201	BCR	C2-C1-C6	3.54	116.01	110.48
14	B4	820	CLA	O2A-CGA-CBA	3.55	122.17	111.92
14	A5	829	CLA	O2A-CGA-CBA	3.55	122.18	111.92
14	A2	1609	CLA	O2A-CGA-CBA	3.55	122.18	111.92
16	A4	844	BCR	C38-C26-C25	3.55	128.48	124.51
14	A4	806	CLA	O2A-CGA-CBA	3.55	122.18	111.92
14	B5	1820	CLA	CMB-C2B-C3B	3.55	131.34	124.88
14	B1	819	CLA	O2A-CGA-CBA	3.55	122.18	111.92
16	J4	103	BCR	C29-C30-C25	3.55	116.03	110.48
14	A3	818	CLA	O2D-CGD-CBD	3.55	117.58	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F6	201	BCR	C2-C1-C6	3.55	116.03	110.48
14	A1	801	CLA	C2C-C1C-NC	3.55	113.77	110.09
14	M1	1201	CLA	O2A-CGA-CBA	3.55	122.19	111.92
14	A6	1627	CLA	O2A-CGA-CBA	3.55	122.19	111.92
14	A5	840	CLA	O2D-CGD-CBD	3.55	117.58	111.28
16	J5	105	BCR	C33-C5-C6	3.55	128.48	124.51
16	A4	849	BCR	C2-C1-C6	3.55	116.03	110.48
14	A1	839	CLA	O2A-CGA-CBA	3.55	122.20	111.92
14	A2	1622	CLA	O2A-CGA-CBA	3.56	122.21	111.92
14	A1	822	CLA	O2A-CGA-CBA	3.56	122.22	111.92
14	B2	821	CLA	O2D-CGD-CBD	3.56	117.60	111.28
14	A5	836	CLA	O2D-CGD-CBD	3.56	117.60	111.28
16	L4	208	BCR	C2-C1-C6	3.56	116.05	110.48
14	A1	818	CLA	O2D-CGD-CBD	3.57	117.60	111.28
14	A4	835	CLA	O2D-CGD-CBD	3.57	117.60	111.28
14	A5	820	CLA	O2A-CGA-CBA	3.57	122.24	111.92
14	A5	823	CLA	O2A-CGA-CBA	3.57	122.24	111.92
14	B2	817	CLA	CMB-C2B-C3B	3.57	131.39	124.88
16	A4	848	BCR	C38-C26-C25	3.58	128.51	124.51
14	B4	830	CLA	C2C-C1C-NC	3.58	113.79	110.09
14	B4	820	CLA	CMB-C2B-C3B	3.58	131.39	124.88
16	B1	848	BCR	C33-C5-C6	3.58	128.51	124.51
14	B1	820	CLA	O2D-CGD-CBD	3.58	117.63	111.28
14	A5	840	CLA	C2C-C1C-NC	3.58	113.80	110.09
14	A3	841	CLA	O2D-CGD-CBD	3.58	117.63	111.28
14	A4	816	CLA	O2D-CGD-CBD	3.58	117.63	111.28
17	X5	102	LHG	O7-C7-C8	3.58	119.10	111.55
16	J3	104	BCR	C2-C1-C6	3.58	116.08	110.48
14	B1	819	CLA	CMB-C2B-C3B	3.58	131.40	124.88
14	B3	1801	CLA	O2A-CGA-CBA	3.58	122.28	111.92
14	A2	1603	CLA	C2C-C1C-NC	3.58	113.80	110.09
14	A1	808	CLA	O2D-CGD-CBD	3.58	117.64	111.28
14	A6	1602	CLA	C2C-C1C-NC	3.58	113.80	110.09
14	B3	1810	CLA	C2C-C1C-NC	3.59	113.80	110.09
14	B2	817	CLA	O2A-CGA-CBA	3.59	122.29	111.92
14	F4	202	CLA	O2D-CGD-CBD	3.59	117.64	111.28
16	F3	201	BCR	C2-C1-C6	3.59	116.09	110.48
14	A2	1611	CLA	O2D-CGD-CBD	3.59	117.65	111.28
14	B4	810	CLA	C2C-C1C-NC	3.59	113.81	110.09
14	A1	837	CLA	C2C-C1C-NC	3.59	113.81	110.09
14	B3	1822	CLA	O2A-CGA-CBA	3.59	122.31	111.92
14	B2	837	CLA	O2D-CGD-CBD	3.59	117.65	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	842	CLA	O2D-CGD-CBD	3.59	117.65	111.28
14	A1	806	CLA	O2D-CGD-CBD	3.59	117.65	111.28
14	B4	819	CLA	O2A-CGA-CBA	3.60	122.32	111.92
14	A1	817	CLA	O2D-CGD-CBD	3.60	117.66	111.28
14	A4	828	CLA	O2A-CGA-CBA	3.60	122.32	111.92
14	B3	1830	CLA	C2C-C1C-NC	3.60	113.81	110.09
14	L6	203	CLA	C2C-C1C-NC	3.60	113.81	110.09
14	A1	816	CLA	O2D-CGD-CBD	3.60	117.66	111.28
14	B5	1830	CLA	C2C-C1C-NC	3.60	113.82	110.09
14	B6	822	CLA	O2D-CGD-CBD	3.60	117.67	111.28
16	L3	201	BCR	C33-C5-C6	3.60	128.54	124.51
16	J1	103	BCR	C29-C30-C25	3.61	116.12	110.48
14	B5	1838	CLA	O2D-CGD-CBD	3.61	117.67	111.28
14	B6	828	CLA	C2C-C1C-NC	3.61	113.82	110.09
14	B5	1819	CLA	O2A-CGA-CBA	3.61	122.35	111.92
14	A1	828	CLA	O2A-CGA-CBA	3.61	122.35	111.92
14	A6	1629	CLA	O2A-CGA-CBA	3.61	122.35	111.92
14	B6	804	CLA	C2C-C1C-NC	3.61	113.83	110.09
16	A1	843	BCR	C2-C1-C6	3.61	116.12	110.48
16	L3	206	BCR	C33-C5-C6	3.61	128.55	124.51
14	A2	1609	CLA	O2D-CGD-CBD	3.61	117.69	111.28
17	A3	853	LHG	C25-C24-C23	3.61	126.64	113.60
14	A4	839	CLA	C2C-C1C-NC	3.61	113.83	110.09
14	A6	1640	CLA	O2D-CGD-CBD	3.61	117.69	111.28
14	A6	1609	CLA	O2D-CGD-CBD	3.61	117.69	111.28
14	A3	841	CLA	C2C-C1C-NC	3.61	113.83	110.09
14	B6	829	CLA	C2C-C1C-NC	3.61	113.83	110.09
14	A3	807	CLA	O2A-CGA-CBA	3.62	122.38	111.92
16	A6	1648	BCR	C2-C1-C6	3.62	116.13	110.48
14	A6	1620	CLA	O2A-CGA-CBA	3.62	122.38	111.92
16	J2	102	BCR	C29-C30-C25	3.62	116.13	110.48
14	B6	818	CLA	O2A-CGA-CBA	3.62	122.38	111.92
14	F3	202	CLA	O2D-CGD-CBD	3.62	117.70	111.28
14	B5	1803	CLA	C2C-C1C-NC	3.62	113.84	110.09
16	A4	845	BCR	C2-C1-C6	3.62	116.14	110.48
14	B4	852	CLA	O2A-CGA-CBA	3.62	122.39	111.92
14	A6	1626	CLA	O2D-CGD-CBD	3.62	117.70	111.28
14	A5	802	CLA	C2C-C1C-NC	3.62	113.84	110.09
14	B1	814	CLA	O2D-CGD-CBD	3.62	117.70	111.28
14	B5	1820	CLA	O2A-CGA-CBA	3.62	122.40	111.92
16	F4	204	BCR	C33-C5-C6	3.62	128.56	124.51
16	J1	103	BCR	C38-C26-C25	3.63	128.57	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	813	CLA	O2D-CGD-CBD	3.63	117.71	111.28
14	A6	1639	CLA	C2C-C1C-NC	3.63	113.85	110.09
14	A5	843	CLA	O2A-CGA-CBA	3.63	122.41	111.92
16	L1	209	BCR	C33-C5-C6	3.63	128.57	124.51
14	B3	1820	CLA	O2A-CGA-CBA	3.63	122.41	111.92
17	B6	849	LHG	O7-C7-C8	3.63	119.20	111.55
16	J2	103	BCR	C2-C1-C6	3.63	116.15	110.48
14	A6	1613	CLA	O2D-CGD-CBD	3.63	117.72	111.28
14	B5	1810	CLA	C2C-C1C-NC	3.63	113.85	110.09
14	B4	807	CLA	C2C-C1C-NC	3.63	113.85	110.09
16	B1	843	BCR	C2-C1-C6	3.63	116.16	110.48
14	A6	1607	CLA	O2A-CGA-CBA	3.63	122.42	111.92
14	B5	1815	CLA	O2D-CGD-CBD	3.63	117.73	111.28
14	F5	1301	CLA	O2D-CGD-CBD	3.64	117.73	111.28
14	A3	829	CLA	O2A-CGA-CBA	3.64	122.44	111.92
16	A3	848	BCR	C2-C1-C6	3.64	116.17	110.48
14	B1	813	CLA	O2D-CGD-CBD	3.64	117.73	111.28
16	A3	851	BCR	C38-C26-C25	3.64	128.58	124.51
14	B6	823	CLA	O2D-CGD-CBD	3.64	117.74	111.28
14	A2	1642	CLA	O2A-CGA-CBA	3.64	122.45	111.92
14	A3	801	CLA	C2C-C1C-NC	3.64	113.86	110.09
14	B2	801	CLA	C2C-C1C-NC	3.64	113.86	110.09
14	B6	820	CLA	O2A-CGA-CBA	3.64	122.46	111.92
16	A1	844	BCR	C29-C30-C25	3.65	116.18	110.48
17	B2	849	LHG	O7-C7-C8	3.65	119.23	111.55
14	B1	821	CLA	O2A-CGA-CBA	3.65	122.48	111.92
14	A3	820	CLA	O2A-CGA-CBA	3.66	122.49	111.92
14	A4	839	CLA	O2A-CGA-CBA	3.66	122.50	111.92
14	B2	828	CLA	C2C-C1C-NC	3.66	113.88	110.09
14	B4	801	CLA	C2C-C1C-NC	3.66	113.88	110.09
14	B6	802	CLA	C2C-C1C-NC	3.66	113.88	110.09
14	A3	802	CLA	C2C-C1C-NC	3.66	113.88	110.09
16	L4	206	BCR	C33-C5-C6	3.66	128.60	124.51
14	F6	202	CLA	O2D-CGD-CBD	3.66	117.77	111.28
16	B5	1845	BCR	C2-C1-C6	3.66	116.20	110.48
14	A1	825	CLA	O2D-CGD-CBD	3.66	117.77	111.28
16	L2	208	BCR	C33-C5-C6	3.66	128.61	124.51
14	B5	1822	CLA	O2A-CGA-CBA	3.66	122.51	111.92
17	A5	852	LHG	O8-C23-C24	3.66	120.99	111.38
14	A6	1618	CLA	O2A-CGA-CBA	3.66	122.52	111.92
14	B2	827	CLA	C2C-C1C-NC	3.67	113.89	110.09
16	F4	201	BCR	C33-C5-C6	3.67	128.61	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A5	847	BCR	C29-C30-C25	3.67	116.21	110.48
14	B4	822	CLA	O2A-CGA-CBA	3.67	122.53	111.92
14	A2	1624	CLA	O2A-CGA-CBA	3.67	122.53	111.92
14	A2	1638	CLA	O2D-CGD-CBD	3.67	117.79	111.28
14	A2	1621	CLA	O2A-CGA-CBA	3.67	122.53	111.92
14	B4	843	CLA	O2D-CGD-CBD	3.67	117.79	111.28
14	B1	853	CLA	O2A-CGA-CBA	3.67	122.54	111.92
16	L5	207	BCR	C33-C5-C6	3.67	128.62	124.51
14	A5	818	CLA	O2A-CGA-CBA	3.67	122.54	111.92
14	B3	1819	CLA	O2A-CGA-CBA	3.67	122.55	111.92
14	A5	841	CLA	O2D-CGD-CBD	3.67	117.80	111.28
14	A4	841	CLA	C2C-C1C-NC	3.67	113.89	110.09
14	B2	819	CLA	O2A-CGA-CBA	3.68	122.56	111.92
14	B2	838	CLA	O2D-CGD-CBD	3.68	117.80	111.28
17	A3	854	LHG	O8-C23-C24	3.68	121.03	111.38
14	B5	1811	CLA	O2D-CGD-CBD	3.68	117.81	111.28
14	A4	820	CLA	CMB-C2B-C3B	3.68	131.59	124.88
14	B6	812	CLA	O2D-CGD-CBD	3.69	117.82	111.28
16	B6	843	BCR	C2-C1-C6	3.69	116.24	110.48
16	L6	201	BCR	C33-C5-C6	3.69	128.64	124.51
16	A4	846	BCR	C29-C30-C25	3.69	116.25	110.48
14	B1	810	CLA	C2C-C1C-NC	3.69	113.91	110.09
14	A1	838	CLA	O2D-CGD-CBD	3.69	117.83	111.28
16	A6	1647	BCR	C38-C26-C25	3.69	128.64	124.51
14	A6	1639	CLA	O2D-CGD-CBD	3.70	117.83	111.28
14	B1	811	CLA	O2D-CGD-CBD	3.70	117.84	111.28
14	A4	825	CLA	O2D-CGD-CBD	3.70	117.84	111.28
14	A4	818	CLA	O2A-CGA-CBA	3.70	122.62	111.92
14	B3	1840	CLA	O2D-CGD-CBD	3.70	117.85	111.28
14	B3	1811	CLA	O2D-CGD-CBD	3.70	117.85	111.28
14	A4	819	CLA	O2A-CGA-CBA	3.70	122.63	111.92
14	A4	839	CLA	O2D-CGD-CBD	3.70	117.85	111.28
14	B1	804	CLA	C2C-C1C-NC	3.70	113.93	110.09
14	B1	801	CLA	C2C-C1C-NC	3.71	113.93	110.09
14	B4	840	CLA	O2D-CGD-CBD	3.71	117.85	111.28
14	A2	1615	CLA	O2D-CGD-CBD	3.71	117.86	111.28
16	B3	1845	BCR	C2-C1-C6	3.71	116.28	110.48
14	A2	1623	CLA	CMB-C2B-C3B	3.71	131.63	124.88
16	A2	1651	BCR	C38-C26-C25	3.71	128.66	124.51
16	L2	201	BCR	C33-C5-C6	3.71	128.66	124.51
14	B4	828	CLA	O2D-CGD-CBD	3.72	117.87	111.28
14	L5	205	CLA	O2D-CGD-CBD	3.72	117.87	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A3	841	CLA	O2A-CGA-CBA	3.72	122.67	111.92
14	A5	807	CLA	O2D-CGD-CBD	3.72	117.88	111.28
16	I1	103	BCR	C33-C5-C6	3.72	128.68	124.51
14	A1	817	CLA	O2A-CGA-CBA	3.72	122.69	111.92
14	B4	829	CLA	O2D-CGD-CBD	3.72	117.89	111.28
14	A5	819	CLA	O2A-CGA-CBA	3.73	122.69	111.92
16	A6	1645	BCR	C29-C30-C25	3.73	116.30	110.48
14	A5	818	CLA	O2D-CGD-CBD	3.73	117.89	111.28
14	A4	812	CLA	O2D-CGD-CBD	3.73	117.89	111.28
14	A1	821	CLA	O2A-CGA-CBA	3.73	122.70	111.92
14	B4	807	CLA	O2D-CGD-CBD	3.73	117.89	111.28
14	B4	811	CLA	O2D-CGD-CBD	3.73	117.89	111.28
14	A3	845	CLA	O2A-CGA-CBA	3.73	122.70	111.92
14	A2	1628	CLA	O2D-CGD-CBD	3.73	117.89	111.28
14	B3	1843	CLA	O2D-CGD-CBD	3.73	117.90	111.28
14	A1	820	CLA	CMB-C2B-C3B	3.73	131.68	124.88
14	L1	201	CLA	O2D-CGD-CBD	3.73	117.90	111.28
14	A1	837	CLA	O2A-CGA-CBA	3.74	122.72	111.92
16	A3	849	BCR	C29-C30-C25	3.74	116.32	110.48
14	A5	822	CLA	O2A-CGA-CBA	3.74	122.75	111.92
14	B2	811	CLA	O2D-CGD-CBD	3.74	117.92	111.28
14	A5	820	CLA	O2D-CGD-CBD	3.75	117.92	111.28
16	B1	852	BCR	C2-C1-C6	3.75	116.34	110.48
14	A1	808	CLA	O2A-CGA-CBA	3.75	122.75	111.92
16	B4	845	BCR	C2-C1-C6	3.75	116.34	110.48
14	A6	1619	CLA	O2A-CGA-CBA	3.75	122.77	111.92
14	A3	843	CLA	C2C-C1C-NC	3.75	113.97	110.09
14	A5	821	CLA	CMB-C2B-C3B	3.75	131.71	124.88
14	B1	829	CLA	C2C-C1C-NC	3.75	113.98	110.09
16	B2	842	BCR	C2-C1-C6	3.75	116.35	110.48
14	A3	816	CLA	O2D-CGD-CBD	3.75	117.94	111.28
14	A5	833	CLA	O2D-CGD-CBD	3.76	117.94	111.28
14	B3	1807	CLA	O2D-CGD-CBD	3.76	117.94	111.28
14	B5	1814	CLA	O2D-CGD-CBD	3.76	117.94	111.28
17	A1	849	LHG	O8-C23-C24	3.76	121.24	111.38
14	A6	1639	CLA	O2A-CGA-CBA	3.76	122.80	111.92
14	A3	819	CLA	O2A-CGA-CBA	3.76	122.80	111.92
14	A4	832	CLA	O2D-CGD-CBD	3.77	117.96	111.28
14	A4	806	CLA	O2D-CGD-CBD	3.77	117.96	111.28
16	L4	208	BCR	C33-C5-C6	3.77	128.73	124.51
14	B3	1829	CLA	O2D-CGD-CBD	3.78	117.98	111.28
14	B1	828	CLA	O2D-CGD-CBD	3.78	117.98	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1622	CLA	O2A-CGA-CBA	3.78	122.85	111.92
14	B4	803	CLA	C2C-C1C-NC	3.78	114.00	110.09
14	A3	818	CLA	O2A-CGA-CBA	3.78	122.86	111.92
14	B1	827	CLA	O2D-CGD-CBD	3.78	117.99	111.28
14	A4	817	CLA	O2A-CGA-CBA	3.79	122.87	111.92
16	J5	103	BCR	C29-C30-C25	3.79	116.40	110.48
14	A1	818	CLA	O2A-CGA-CBA	3.79	122.88	111.92
14	A4	831	CLA	O2D-CGD-CBD	3.79	118.00	111.28
14	B3	1804	CLA	C2C-C1C-NC	3.79	114.01	110.09
14	A3	821	CLA	CMB-C2B-C3B	3.79	131.78	124.88
14	A4	821	CLA	O2A-CGA-CBA	3.79	122.88	111.92
14	A4	840	CLA	O2D-CGD-CBD	3.80	118.01	111.28
14	F1	1301	CLA	O2D-CGD-CBD	3.80	118.01	111.28
14	A5	836	CLA	O2A-CGA-CBA	3.80	122.90	111.92
14	A6	1636	CLA	O2A-CGA-CBA	3.80	122.90	111.92
14	B4	820	CLA	O2D-CGD-CBD	3.80	118.02	111.28
14	A6	1616	CLA	O2D-CGD-CBD	3.80	118.02	111.28
14	B3	1803	CLA	C2C-C1C-NC	3.80	114.03	110.09
14	B3	1842	CLA	C2C-C1C-NC	3.80	114.03	110.09
14	A2	1622	CLA	O2D-CGD-CBD	3.81	118.03	111.28
14	B6	809	CLA	O2D-CGD-CBD	3.81	118.04	111.28
14	A5	826	CLA	O2D-CGD-CBD	3.81	118.04	111.28
14	A3	822	CLA	O2A-CGA-CBA	3.81	122.94	111.92
14	B2	840	CLA	O2D-CGD-CBD	3.81	118.04	111.28
14	A5	832	CLA	O2D-CGD-CBD	3.81	118.04	111.28
14	A1	815	CLA	O2D-CGD-CBD	3.82	118.05	111.28
14	L6	202	CLA	O2D-CGD-CBD	3.82	118.05	111.28
14	A6	1621	CLA	CMB-C2B-C3B	3.82	131.83	124.88
14	B6	841	CLA	O2D-CGD-CBD	3.82	118.05	111.28
14	A5	840	CLA	O2A-CGA-CBA	3.82	122.96	111.92
14	B2	817	CLA	O2D-CGD-CBD	3.82	118.05	111.28
14	B5	1828	CLA	O2D-CGD-CBD	3.82	118.06	111.28
14	A1	819	CLA	O2D-CGD-CBD	3.82	118.06	111.28
14	A2	1620	CLA	O2A-CGA-CBA	3.82	122.97	111.92
14	A1	831	CLA	O2D-CGD-CBD	3.82	118.06	111.28
14	A3	805	CLA	O2D-CGD-CBD	3.83	118.06	111.28
16	B3	1851	BCR	C33-C5-C6	3.83	128.79	124.51
14	B2	808	CLA	C2C-C1C-NC	3.83	114.05	110.09
14	A5	842	CLA	C2C-C1C-NC	3.83	114.06	110.09
14	A3	809	CLA	O2A-CGA-CBA	3.83	123.00	111.92
14	A1	836	CLA	O2A-CGA-CBA	3.83	123.00	111.92
14	B2	808	CLA	O2D-CGD-CBD	3.84	118.08	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B3	1814	CLA	O2D-CGD-CBD	3.84	118.08	111.28
14	A4	819	CLA	O2D-CGD-CBD	3.84	118.09	111.28
14	A3	837	CLA	O2A-CGA-CBA	3.84	123.03	111.92
17	A6	1649	LHG	C25-C24-C23	3.84	127.47	113.60
14	B4	825	CLA	O2D-CGD-CBD	3.84	118.10	111.28
14	B1	841	CLA	O2D-CGD-CBD	3.85	118.10	111.28
14	A6	1609	CLA	O2A-CGA-CBA	3.85	123.04	111.92
14	A2	1638	CLA	O2A-CGA-CBA	3.85	123.05	111.92
14	B5	1825	CLA	O2D-CGD-CBD	3.85	118.10	111.28
14	A1	839	CLA	C2C-C1C-NC	3.85	114.08	110.09
14	A4	835	CLA	O2A-CGA-CBA	3.85	123.05	111.92
14	B5	1842	CLA	C2C-C1C-NC	3.85	114.08	110.09
14	B2	825	CLA	O2D-CGD-CBD	3.85	118.11	111.28
14	A4	808	CLA	O2A-CGA-CBA	3.85	123.07	111.92
16	A2	1649	BCR	C29-C30-C25	3.86	116.51	110.48
14	A1	828	CLA	O2D-CGD-CBD	3.86	118.12	111.28
14	B2	807	CLA	O2A-CGA-CBA	3.86	123.08	111.92
14	B4	814	CLA	O2D-CGD-CBD	3.86	118.12	111.28
14	B4	841	CLA	O2D-CGD-CBD	3.86	118.13	111.28
14	L1	206	CLA	O2D-CGD-CBD	3.87	118.14	111.28
14	A5	809	CLA	O2A-CGA-CBA	3.87	123.11	111.92
14	B5	1807	CLA	O2D-CGD-CBD	3.88	118.15	111.28
14	A5	838	CLA	O2A-CGA-CBA	3.88	123.14	111.92
14	A2	1635	CLA	C2C-C1C-NC	3.88	114.11	110.09
14	A6	1612	CLA	O2D-CGD-CBD	3.88	118.17	111.28
14	B4	830	CLA	O2A-CGA-CBA	3.88	123.15	111.92
14	I1	101	CLA	C2C-C1C-NC	3.89	114.12	110.09
16	B3	1851	BCR	C2-C1-C6	3.89	116.56	110.48
14	B3	1825	CLA	O2D-CGD-CBD	3.89	118.18	111.28
14	B1	838	CLA	O2D-CGD-CBD	3.89	118.18	111.28
14	B1	829	CLA	O2A-CGA-CBA	3.89	123.17	111.92
14	A5	802	CLA	O2D-CGD-CBD	3.90	118.19	111.28
14	A3	839	CLA	O2A-CGA-CBA	3.90	123.19	111.92
14	A6	1620	CLA	O2D-CGD-CBD	3.90	118.19	111.28
14	B5	1843	CLA	O2D-CGD-CBD	3.90	118.19	111.28
14	A6	1632	CLA	O2D-CGD-CBD	3.90	118.20	111.28
14	A1	837	CLA	O2D-CGD-CBD	3.90	118.20	111.28
14	A5	812	CLA	O2D-CGD-CBD	3.90	118.20	111.28
14	B2	826	CLA	O2D-CGD-CBD	3.90	118.20	111.28
14	A1	804	CLA	O2D-CGD-CBD	3.91	118.21	111.28
14	A2	1618	CLA	O2D-CGD-CBD	3.91	118.21	111.28
14	A4	832	CLA	C2C-C1C-NC	3.91	114.14	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A6	1651	CLA	C2C-C1C-NC	3.91	114.14	110.09
14	B5	1804	CLA	C2C-C1C-NC	3.91	114.14	110.09
14	B6	808	CLA	O2A-CGA-CBA	3.91	123.23	111.92
14	A1	813	CLA	O2D-CGD-CBD	3.91	118.22	111.28
17	A6	1650	LHG	O8-C23-C24	3.92	121.65	111.38
14	B3	1810	CLA	O2A-CGA-CBA	3.92	123.25	111.92
14	A4	835	CLA	C2C-C1C-NC	3.92	114.15	110.09
14	B3	1841	CLA	O2D-CGD-CBD	3.92	118.23	111.28
14	B1	805	CLA	C2C-C1C-NC	3.92	114.15	110.09
14	B3	1828	CLA	O2D-CGD-CBD	3.92	118.24	111.28
14	A2	1635	CLA	O2D-CGD-CBD	3.93	118.24	111.28
14	B6	806	CLA	O2D-CGD-CBD	3.93	118.24	111.28
14	A1	834	CLA	O2A-CGA-CBA	3.93	123.28	111.92
14	B1	811	CLA	C2C-C1C-NC	3.93	114.16	110.09
16	B2	850	BCR	C2-C1-C6	3.93	116.63	110.48
14	B5	1830	CLA	O2A-CGA-CBA	3.93	123.29	111.92
14	B6	840	CLA	C2C-C1C-NC	3.93	114.16	110.09
14	A1	833	CLA	O2D-CGD-CBD	3.93	118.26	111.28
14	B4	810	CLA	O2A-CGA-CBA	3.94	123.30	111.92
14	L2	207	CLA	O2D-CGD-CBD	3.94	118.26	111.28
14	A3	812	CLA	O2D-CGD-CBD	3.94	118.26	111.28
14	A2	1611	CLA	O2A-CGA-CBA	3.94	123.31	111.92
14	B2	839	CLA	C2C-C1C-NC	3.94	114.17	110.09
14	B6	813	CLA	O2D-CGD-CBD	3.94	118.27	111.28
14	A5	833	CLA	C2C-C1C-NC	3.94	114.17	110.09
14	L4	204	CLA	O2D-CGD-CBD	3.94	118.27	111.28
14	A4	815	CLA	O2D-CGD-CBD	3.94	118.28	111.28
14	B3	1838	CLA	O2D-CGD-CBD	3.94	118.28	111.28
14	B5	1829	CLA	O2D-CGD-CBD	3.95	118.28	111.28
14	B4	838	CLA	O2D-CGD-CBD	3.95	118.28	111.28
14	A2	1642	CLA	O2D-CGD-CBD	3.95	118.28	111.28
14	X6	1701	CLA	O2D-CGD-CBD	3.95	118.28	111.28
14	A1	811	CLA	O2D-CGD-CBD	3.95	118.28	111.28
17	A1	848	LHG	C25-C24-C23	3.95	127.86	113.60
14	A6	1629	CLA	O2D-CGD-CBD	3.95	118.29	111.28
14	B2	802	CLA	C2C-C1C-NC	3.96	114.19	110.09
14	A5	829	CLA	O2D-CGD-CBD	3.96	118.30	111.28
14	B1	837	CLA	O2D-CGD-CBD	3.96	118.30	111.28
14	A6	1603	CLA	O2A-CGA-CBA	3.96	123.37	111.92
14	B6	836	CLA	O2D-CGD-CBD	3.96	118.30	111.28
14	B3	1811	CLA	C2C-C1C-NC	3.96	114.19	110.09
14	A4	837	CLA	O2A-CGA-CBA	3.96	123.38	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1840	CLA	O2D-CGD-CBD	3.96	118.31	111.28
14	B4	815	CLA	O2D-CGD-CBD	3.96	118.31	111.28
14	A3	802	CLA	O2D-CGD-CBD	3.97	118.32	111.28
14	B1	817	CLA	O2D-CGD-CBD	3.97	118.32	111.28
14	L2	206	CLA	O2D-CGD-CBD	3.97	118.32	111.28
14	A3	832	CLA	O2D-CGD-CBD	3.97	118.32	111.28
14	B6	826	CLA	O2D-CGD-CBD	3.98	118.33	111.28
14	A2	1607	CLA	O2D-CGD-CBD	3.98	118.33	111.28
14	X3	102	CLA	O2D-CGD-CBD	3.98	118.33	111.28
14	A1	834	CLA	C2C-C1C-NC	3.98	114.21	110.09
14	A3	833	CLA	O2D-CGD-CBD	3.99	118.35	111.28
14	A2	1604	CLA	O2A-CGA-CBA	3.99	123.45	111.92
14	B1	839	CLA	O2D-CGD-CBD	3.99	118.35	111.28
14	B5	1810	CLA	O2A-CGA-CBA	3.99	123.46	111.92
14	X4	102	CLA	O2D-CGD-CBD	3.99	118.36	111.28
14	A1	831	CLA	C2C-C1C-NC	3.99	114.22	110.09
14	B2	822	CLA	O2D-CGD-CBD	3.99	118.36	111.28
14	A2	1638	CLA	C2C-C1C-NC	4.00	114.23	110.09
14	B3	1802	CLA	O2A-CGA-CBA	4.00	123.48	111.92
14	B2	804	CLA	O2D-CGD-CBD	4.00	118.37	111.28
14	A2	1640	CLA	O2A-CGA-CBA	4.00	123.49	111.92
14	A2	1631	CLA	O2D-CGD-CBD	4.00	118.38	111.28
14	B1	807	CLA	O2D-CGD-CBD	4.00	118.38	111.28
14	B6	828	CLA	O2A-CGA-CBA	4.00	123.50	111.92
14	L6	207	CLA	O2D-CGD-CBD	4.01	118.38	111.28
14	A3	829	CLA	O2D-CGD-CBD	4.01	118.39	111.28
14	A3	820	CLA	O2D-CGD-CBD	4.01	118.39	111.28
16	F4	204	BCR	C2-C1-C6	4.01	116.75	110.48
14	A2	1614	CLA	O2D-CGD-CBD	4.01	118.39	111.28
17	A2	1653	LHG	C25-C24-C23	4.01	128.07	113.60
14	A5	809	CLA	O2D-CGD-CBD	4.01	118.39	111.28
14	B1	810	CLA	O2A-CGA-CBA	4.01	123.53	111.92
14	A3	833	CLA	C2C-C1C-NC	4.01	114.25	110.09
19	B2	848	LMG	C30-C29-C28	4.01	128.09	113.60
19	B5	1851	LMG	C30-C29-C28	4.02	128.09	113.60
14	B4	842	CLA	C2C-C1C-NC	4.02	114.25	110.09
14	A5	816	CLA	O2D-CGD-CBD	4.02	118.41	111.28
14	A6	1638	CLA	O2A-CGA-CBA	4.02	123.55	111.92
14	B5	1811	CLA	C2C-C1C-NC	4.03	114.26	110.09
16	B2	843	BCR	C38-C26-C25	4.03	129.01	124.51
14	B5	1841	CLA	O2D-CGD-CBD	4.03	118.42	111.28
14	B2	835	CLA	O2D-CGD-CBD	4.03	118.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	809	CLA	C2C-C1C-NC	4.04	114.27	110.09
16	B1	844	BCR	C38-C26-C25	4.04	129.03	124.51
14	B3	1839	CLA	O2D-CGD-CBD	4.04	118.44	111.28
14	B3	1815	CLA	O2D-CGD-CBD	4.04	118.44	111.28
14	B4	811	CLA	C2C-C1C-NC	4.04	114.27	110.09
14	B3	1830	CLA	O2A-CGA-CBA	4.04	123.60	111.92
14	L4	205	CLA	O2D-CGD-CBD	4.04	118.45	111.28
14	B4	802	CLA	O2A-CGA-CBA	4.04	123.62	111.92
19	B1	850	LMG	C30-C29-C28	4.05	128.20	113.60
17	A4	850	LHG	C25-C24-C23	4.05	128.21	113.60
19	B6	848	LMG	C30-C29-C28	4.05	128.22	113.60
16	J5	105	BCR	C2-C1-C6	4.05	116.81	110.48
14	A5	805	CLA	O2D-CGD-CBD	4.05	118.47	111.28
14	L1	207	CLA	O2D-CGD-CBD	4.05	118.47	111.28
17	A5	851	LHG	C25-C24-C23	4.05	128.23	113.60
19	B4	851	LMG	C30-C29-C28	4.05	128.23	113.60
14	B2	827	CLA	O2A-CGA-CBA	4.06	123.65	111.92
14	A6	1632	CLA	C2C-C1C-NC	4.06	114.29	110.09
14	A2	1627	CLA	O2D-CGD-CBD	4.06	118.48	111.28
14	A4	828	CLA	O2D-CGD-CBD	4.06	118.48	111.28
14	L3	205	CLA	O2D-CGD-CBD	4.06	118.48	111.28
14	B2	815	CLA	O2D-CGD-CBD	4.06	118.48	111.28
14	A3	837	CLA	C2C-C1C-NC	4.07	114.30	110.09
14	B6	827	CLA	O2D-CGD-CBD	4.07	118.49	111.28
16	B6	844	BCR	C38-C26-C25	4.07	129.06	124.51
14	A3	825	CLA	O2D-CGD-CBD	4.07	118.51	111.28
14	A4	813	CLA	O2D-CGD-CBD	4.09	118.53	111.28
14	A2	1603	CLA	O2D-CGD-CBD	4.09	118.53	111.28
14	A3	814	CLA	O2D-CGD-CBD	4.09	118.53	111.28
14	B2	812	CLA	O2D-CGD-CBD	4.09	118.54	111.28
14	B5	1818	CLA	O2D-CGD-CBD	4.10	118.54	111.28
19	B3	1850	LMG	C30-C29-C28	4.10	128.38	113.60
14	B6	837	CLA	O2D-CGD-CBD	4.10	118.55	111.28
16	B5	1846	BCR	C38-C26-C25	4.10	129.10	124.51
14	B6	838	CLA	O2D-CGD-CBD	4.10	118.55	111.28
14	B6	839	CLA	O2D-CGD-CBD	4.10	118.55	111.28
14	B5	1833	CLA	O2D-CGD-CBD	4.10	118.56	111.28
14	B1	819	CLA	O2D-CGD-CBD	4.11	118.57	111.28
16	I4	101	BCR	C2-C1-C6	4.11	116.91	110.48
14	B5	1820	CLA	O2D-CGD-CBD	4.12	118.59	111.28
14	B1	801	CLA	O2D-CGD-CBD	4.13	118.60	111.28
14	X2	1701	CLA	O2D-CGD-CBD	4.13	118.60	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	802	CLA	O2D-CGD-CBD	4.13	118.61	111.28
14	B4	826	CLA	O2D-CGD-CBD	4.13	118.61	111.28
16	B6	843	BCR	C38-C26-C25	4.14	129.14	124.51
16	B6	850	BCR	C2-C1-C6	4.14	116.94	110.48
14	X1	1701	CLA	O2D-CGD-CBD	4.14	118.61	111.28
14	B1	832	CLA	O2D-CGD-CBD	4.14	118.63	111.28
14	A6	1605	CLA	O2D-CGD-CBD	4.14	118.63	111.28
14	B2	836	CLA	O2D-CGD-CBD	4.15	118.63	111.28
14	B6	818	CLA	O2D-CGD-CBD	4.15	118.64	111.28
14	B1	825	CLA	O2D-CGD-CBD	4.15	118.64	111.28
14	A4	804	CLA	O2D-CGD-CBD	4.15	118.64	111.28
14	A6	1614	CLA	O2D-CGD-CBD	4.15	118.64	111.28
14	B4	804	CLA	C2C-C1C-NC	4.16	114.39	110.09
16	I2	101	BCR	C2-C1-C6	4.16	116.98	110.48
14	B5	1802	CLA	O2A-CGA-CBA	4.16	123.95	111.92
14	A6	1635	CLA	O2D-CGD-CBD	4.16	118.66	111.28
14	A2	1634	CLA	O2D-CGD-CBD	4.17	118.67	111.28
14	A5	841	CLA	O2A-CGA-CBA	4.17	123.97	111.92
14	B1	840	CLA	O2D-CGD-CBD	4.17	118.67	111.28
14	B3	1818	CLA	O2D-CGD-CBD	4.17	118.67	111.28
14	A2	1643	CLA	O2A-CGA-CBA	4.17	123.98	111.92
14	A5	836	CLA	C2C-C1C-NC	4.17	114.41	110.09
14	A4	840	CLA	O2A-CGA-CBA	4.18	124.00	111.92
14	B1	802	CLA	O2A-CGA-CBA	4.18	124.02	111.92
14	B3	1826	CLA	O2D-CGD-CBD	4.19	118.72	111.28
14	J5	101	CLA	O2D-CGD-CBD	4.20	118.72	111.28
16	B4	846	BCR	C38-C26-C25	4.20	129.21	124.51
14	A2	1616	CLA	O2D-CGD-CBD	4.20	118.73	111.28
14	A4	802	CLA	O2D-CGD-CBD	4.20	118.73	111.28
14	A2	1637	CLA	O2D-CGD-CBD	4.20	118.73	111.28
14	B6	816	CLA	O2D-CGD-CBD	4.21	118.74	111.28
14	J4	101	CLA	O2D-CGD-CBD	4.21	118.74	111.28
14	A4	811	CLA	O2D-CGD-CBD	4.21	118.74	111.28
14	L3	204	CLA	O2D-CGD-CBD	4.21	118.74	111.28
14	B4	818	CLA	O2D-CGD-CBD	4.21	118.75	111.28
14	A6	1636	CLA	C2C-C1C-NC	4.21	114.45	110.09
14	B5	1839	CLA	O2D-CGD-CBD	4.21	118.75	111.28
14	J6	1102	CLA	O2D-CGD-CBD	4.22	118.76	111.28
14	A3	842	CLA	O2A-CGA-CBA	4.22	124.12	111.92
16	A3	852	BCR	C40-C30-C25	4.22	117.16	110.31
14	B4	839	CLA	O2D-CGD-CBD	4.23	118.77	111.28
14	B5	1826	CLA	O2D-CGD-CBD	4.23	118.77	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B3	1820	CLA	O2D-CGD-CBD	4.23	118.78	111.28
14	B4	801	CLA	O2D-CGD-CBD	4.23	118.78	111.28
16	B3	1846	BCR	C38-C26-C25	4.23	129.25	124.51
14	A5	814	CLA	O2D-CGD-CBD	4.24	118.81	111.28
14	B2	833	CLA	O2D-CGD-CBD	4.25	118.82	111.28
14	A1	824	CLA	O2D-CGD-CBD	4.26	118.83	111.28
16	I6	102	BCR	C2-C1-C6	4.27	117.15	110.48
16	B5	1845	BCR	C38-C26-C25	4.27	129.28	124.51
14	A5	835	CLA	O2D-CGD-CBD	4.27	118.85	111.28
16	A1	847	BCR	C40-C30-C25	4.27	117.23	110.31
16	B1	843	BCR	C38-C26-C25	4.27	129.29	124.51
14	A5	825	CLA	O2D-CGD-CBD	4.27	118.85	111.28
16	A4	849	BCR	C40-C30-C25	4.27	117.23	110.31
14	B6	834	CLA	O2D-CGD-CBD	4.27	118.86	111.28
14	B1	835	CLA	O2D-CGD-CBD	4.28	118.86	111.28
16	I3	101	BCR	C2-C1-C6	4.28	117.17	110.48
16	I1	102	BCR	C2-C1-C6	4.28	117.17	110.48
14	A1	838	CLA	O2A-CGA-CBA	4.28	124.31	111.92
14	B2	823	CLA	O2D-CGD-CBD	4.28	118.88	111.28
14	B2	819	CLA	O2D-CGD-CBD	4.29	118.88	111.28
14	A6	1627	CLA	O2D-CGD-CBD	4.29	118.88	111.28
14	A6	1640	CLA	O2A-CGA-CBA	4.29	124.32	111.92
16	A2	1652	BCR	C40-C30-C25	4.29	117.27	110.31
14	A1	807	CLA	O2D-CGD-CBD	4.29	118.89	111.28
14	B3	1832	CLA	O2D-CGD-CBD	4.30	118.90	111.28
14	A6	1625	CLA	O2D-CGD-CBD	4.30	118.90	111.28
14	B1	831	CLA	O2D-CGD-CBD	4.30	118.91	111.28
14	K3	1401	CLA	O2D-CGD-CBD	4.30	118.91	111.28
14	B4	823	CLA	O2D-CGD-CBD	4.31	118.92	111.28
14	B4	812	CLA	C2C-C1C-NC	4.31	114.55	110.09
16	A6	1648	BCR	C40-C30-C25	4.31	117.30	110.31
14	B6	824	CLA	O2D-CGD-CBD	4.31	118.92	111.28
14	A4	834	CLA	O2D-CGD-CBD	4.31	118.93	111.28
14	B5	1836	CLA	O2D-CGD-CBD	4.31	118.93	111.28
14	A3	836	CLA	O2D-CGD-CBD	4.32	118.94	111.28
14	X5	101	CLA	O2D-CGD-CBD	4.32	118.94	111.28
14	B4	836	CLA	O2D-CGD-CBD	4.32	118.94	111.28
14	B6	821	CLA	O2D-CGD-CBD	4.33	118.96	111.28
14	A6	1622	CLA	O2D-CGD-CBD	4.33	118.96	111.28
14	B3	1823	CLA	O2D-CGD-CBD	4.33	118.97	111.28
14	L6	208	CLA	O2D-CGD-CBD	4.34	118.97	111.28
16	A5	850	BCR	C40-C30-C25	4.34	117.34	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L5	206	CLA	O2D-CGD-CBD	4.34	118.97	111.28
14	A2	1605	CLA	O2D-CGD-CBD	4.34	118.98	111.28
14	A3	823	CLA	O2D-CGD-CBD	4.34	118.98	111.28
14	B1	822	CLA	O2D-CGD-CBD	4.34	118.98	111.28
14	A4	824	CLA	O2D-CGD-CBD	4.35	118.99	111.28
14	B5	1812	CLA	C2C-C1C-NC	4.36	114.60	110.09
14	A1	821	CLA	O2D-CGD-CBD	4.36	119.01	111.28
14	J1	101	CLA	O2D-CGD-CBD	4.36	119.01	111.28
14	B6	827	CLA	O2A-CGA-CBA	4.36	124.53	111.92
14	J3	101	CLA	O2D-CGD-CBD	4.36	119.02	111.28
16	B4	845	BCR	C38-C26-C25	4.36	129.39	124.51
14	B2	831	CLA	O2D-CGD-CBD	4.37	119.03	111.28
14	B3	1833	CLA	O2D-CGD-CBD	4.37	119.03	111.28
14	A2	1629	CLA	O2D-CGD-CBD	4.37	119.04	111.28
14	A5	822	CLA	O2D-CGD-CBD	4.37	119.04	111.28
14	A3	831	CLA	O2D-CGD-CBD	4.38	119.04	111.28
16	B3	1845	BCR	C38-C26-C25	4.38	129.42	124.51
14	B3	1836	CLA	O2D-CGD-CBD	4.39	119.07	111.28
14	M3	1601	CLA	O2D-CGD-CBD	4.40	119.08	111.28
14	A4	837	CLA	O2D-CGD-CBD	4.40	119.08	111.28
14	B2	820	CLA	O2D-CGD-CBD	4.40	119.08	111.28
14	B6	832	CLA	O2D-CGD-CBD	4.40	119.08	111.28
14	A5	823	CLA	O2D-CGD-CBD	4.40	119.08	111.28
14	A5	827	CLA	O2D-CGD-CBD	4.40	119.09	111.28
14	A2	1601	CLA	O2D-CGD-CBD	4.40	119.09	111.28
14	A3	822	CLA	O2D-CGD-CBD	4.41	119.09	111.28
14	B1	828	CLA	O2A-CGA-CBA	4.41	124.67	111.92
14	J2	101	CLA	O2D-CGD-CBD	4.41	119.10	111.28
16	I5	101	BCR	C2-C1-C6	4.42	117.39	110.48
16	B4	847	BCR	C29-C30-C25	4.43	117.41	110.48
14	A2	1640	CLA	O2D-CGD-CBD	4.43	119.14	111.28
14	B5	1822	CLA	O2D-CGD-CBD	4.43	119.14	111.28
14	A4	826	CLA	O2D-CGD-CBD	4.43	119.14	111.28
14	A3	808	CLA	O2D-CGD-CBD	4.44	119.15	111.28
14	A1	836	CLA	O2D-CGD-CBD	4.44	119.15	111.28
14	B2	830	CLA	O2D-CGD-CBD	4.44	119.15	111.28
14	K4	1401	CLA	O2D-CGD-CBD	4.45	119.17	111.28
14	B5	1829	CLA	O2A-CGA-CBA	4.45	124.79	111.92
14	A1	802	CLA	O2D-CGD-CBD	4.45	119.18	111.28
14	A4	822	CLA	O2D-CGD-CBD	4.45	119.18	111.28
14	B6	831	CLA	O2D-CGD-CBD	4.46	119.18	111.28
14	B1	854	CLA	C2C-C1C-NC	4.46	114.71	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B3	1822	CLA	O2D-CGD-CBD	4.46	119.19	111.28
16	B1	845	BCR	C29-C30-C25	4.46	117.46	110.48
15	B3	1844	PQN	C14-C13-C15	4.47	122.99	115.29
14	K5	102	CLA	O2D-CGD-CBD	4.47	119.21	111.28
14	A2	1624	CLA	O2D-CGD-CBD	4.47	119.21	111.28
14	A1	826	CLA	O2D-CGD-CBD	4.48	119.22	111.28
14	A3	827	CLA	O2D-CGD-CBD	4.48	119.23	111.28
14	A5	803	CLA	O2D-CGD-CBD	4.48	119.23	111.28
14	A4	830	CLA	O2D-CGD-CBD	4.48	119.23	111.28
14	I6	101	CLA	O2D-CGD-CBD	4.48	119.23	111.28
14	B4	829	CLA	O2A-CGA-CBA	4.49	124.90	111.92
16	B5	1847	BCR	C29-C30-C25	4.49	117.50	110.48
16	B3	1847	BCR	C29-C30-C25	4.49	117.50	110.48
14	B2	809	CLA	C2C-C1C-NC	4.50	114.75	110.09
15	B1	842	PQN	C14-C13-C15	4.50	123.05	115.29
14	B6	810	CLA	C2C-C1C-NC	4.50	114.75	110.09
14	B5	1823	CLA	O2D-CGD-CBD	4.50	119.26	111.28
14	B1	826	CLA	O2D-CGD-CBD	4.50	119.26	111.28
14	B4	822	CLA	O2D-CGD-CBD	4.50	119.27	111.28
15	B6	842	PQN	C14-C13-C15	4.51	123.06	115.29
14	K6	1401	CLA	O2D-CGD-CBD	4.51	119.28	111.28
14	A6	1623	CLA	O2D-CGD-CBD	4.51	119.28	111.28
14	J6	1101	CLA	O2D-CGD-CBD	4.51	119.28	111.28
14	A1	822	CLA	O2D-CGD-CBD	4.51	119.28	111.28
14	A3	839	CLA	O2D-CGD-CBD	4.52	119.30	111.28
14	A6	1608	CLA	O2D-CGD-CBD	4.53	119.32	111.28
14	A4	821	CLA	O2D-CGD-CBD	4.53	119.32	111.28
14	B3	1812	CLA	C2C-C1C-NC	4.53	114.78	110.09
14	B3	1834	CLA	O2D-CGD-CBD	4.53	119.32	111.28
15	B4	844	PQN	C14-C13-C15	4.53	123.11	115.29
14	B3	1829	CLA	O2A-CGA-CBA	4.54	125.05	111.92
14	K2	1401	CLA	O2D-CGD-CBD	4.54	119.33	111.28
14	A3	803	CLA	O2D-CGD-CBD	4.55	119.34	111.28
14	A4	853	CLA	O2D-CGD-CBD	4.55	119.34	111.28
16	B6	845	BCR	C29-C30-C25	4.55	117.59	110.48
14	A1	830	CLA	O2D-CGD-CBD	4.55	119.35	111.28
16	B2	844	BCR	C29-C30-C25	4.55	117.60	110.48
14	B2	806	CLA	O2D-CGD-CBD	4.55	119.35	111.28
14	A5	808	CLA	O2D-CGD-CBD	4.56	119.37	111.28
16	B2	842	BCR	C38-C26-C25	4.56	129.62	124.51
14	A2	1632	CLA	O2D-CGD-CBD	4.57	119.38	111.28
14	B3	1809	CLA	O2D-CGD-CBD	4.57	119.39	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B4	833	CLA	O2D-CGD-CBD	4.57	119.39	111.28
14	B5	1827	CLA	O2D-CGD-CBD	4.57	119.39	111.28
14	B2	826	CLA	O2A-CGA-CBA	4.57	125.15	111.92
14	A2	1625	CLA	O2D-CGD-CBD	4.58	119.39	111.28
14	L3	202	CLA	O2D-CGD-CBD	4.58	119.40	111.28
14	B4	834	CLA	O2D-CGD-CBD	4.59	119.41	111.28
14	B5	1832	CLA	O2D-CGD-CBD	4.59	119.41	111.28
14	A6	1630	CLA	O2D-CGD-CBD	4.59	119.42	111.28
14	K1	1401	CLA	O2D-CGD-CBD	4.59	119.42	111.28
14	B2	829	CLA	O2D-CGD-CBD	4.60	119.44	111.28
14	A4	807	CLA	O2D-CGD-CBD	4.60	119.44	111.28
14	A6	1638	CLA	O2D-CGD-CBD	4.61	119.45	111.28
14	A3	806	CLA	O2A-CGA-CBA	4.61	125.25	111.92
15	B2	841	PQN	C14-C13-C15	4.61	123.25	115.29
14	B5	1809	CLA	O2D-CGD-CBD	4.62	119.47	111.28
14	A4	829	CLA	O2D-CGD-CBD	4.62	119.47	111.28
14	B3	1835	CLA	O2D-CGD-CBD	4.63	119.48	111.28
14	A5	830	CLA	O2D-CGD-CBD	4.63	119.49	111.28
14	B6	830	CLA	O2D-CGD-CBD	4.63	119.49	111.28
15	B5	1844	PQN	C14-C13-C15	4.64	123.28	115.29
14	A2	1633	CLA	O2D-CGD-CBD	4.64	119.51	111.28
14	A6	1601	CLA	O2D-CGD-CBD	4.64	119.51	111.28
14	B4	832	CLA	O2D-CGD-CBD	4.64	119.52	111.28
14	A3	830	CLA	O2D-CGD-CBD	4.65	119.53	111.28
14	B5	1834	CLA	O2D-CGD-CBD	4.67	119.56	111.28
14	B6	833	CLA	O2D-CGD-CBD	4.67	119.57	111.28
14	B4	817	CLA	O2D-CGD-CBD	4.68	119.58	111.28
14	B2	813	CLA	O2D-CGD-CBD	4.69	119.59	111.28
14	A2	1617	CLA	O2D-CGD-CBD	4.70	119.61	111.28
14	B3	1816	CLA	O2D-CGD-CBD	4.70	119.61	111.28
14	A3	815	CLA	O2D-CGD-CBD	4.70	119.61	111.28
14	B1	821	CLA	O2D-CGD-CBD	4.70	119.61	111.28
14	A1	829	CLA	O2D-CGD-CBD	4.71	119.63	111.28
14	B4	852	CLA	O2D-CGD-CBD	4.71	119.64	111.28
14	B1	809	CLA	O2D-CGD-CBD	4.72	119.66	111.28
14	B5	1817	CLA	O2D-CGD-CBD	4.72	119.66	111.28
14	A2	1610	CLA	O2D-CGD-CBD	4.73	119.66	111.28
14	B4	835	CLA	O2D-CGD-CBD	4.73	119.67	111.28
14	A5	838	CLA	O2D-CGD-CBD	4.74	119.68	111.28
14	L5	202	CLA	O2D-CGD-CBD	4.75	119.70	111.28
14	L5	204	CLA	O2D-CGD-CBD	4.75	119.71	111.28
14	B4	831	CLA	O2D-CGD-CBD	4.76	119.71	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B6	815	CLA	O2D-CGD-CBD	4.76	119.72	111.28
14	A5	815	CLA	O2D-CGD-CBD	4.76	119.72	111.28
14	A1	814	CLA	O2D-CGD-CBD	4.77	119.73	111.28
14	A6	1631	CLA	O2D-CGD-CBD	4.77	119.74	111.28
14	B4	816	CLA	O2D-CGD-CBD	4.77	119.75	111.28
14	A5	831	CLA	O2D-CGD-CBD	4.78	119.76	111.28
14	L4	203	CLA	O2D-CGD-CBD	4.79	119.78	111.28
14	A6	1606	CLA	O2A-CGA-CBA	4.79	125.79	111.92
14	B4	809	CLA	O2D-CGD-CBD	4.80	119.79	111.28
14	B5	1831	CLA	O2D-CGD-CBD	4.80	119.79	111.28
14	B2	832	CLA	O2D-CGD-CBD	4.80	119.79	111.28
14	B1	816	CLA	O2D-CGD-CBD	4.80	119.80	111.28
14	B2	814	CLA	O2D-CGD-CBD	4.82	119.83	111.28
14	A6	1615	CLA	O2D-CGD-CBD	4.83	119.84	111.28
14	A4	814	CLA	O2D-CGD-CBD	4.83	119.85	111.28
14	L1	205	CLA	O2D-CGD-CBD	4.84	119.86	111.28
14	B1	815	CLA	O2D-CGD-CBD	4.84	119.87	111.28
14	A2	1608	CLA	O2A-CGA-CBA	4.85	125.95	111.92
14	B6	820	CLA	O2D-CGD-CBD	4.86	119.89	111.28
14	B6	808	CLA	O2D-CGD-CBD	4.87	119.92	111.28
14	B3	1827	CLA	O2D-CGD-CBD	4.88	119.94	111.28
14	B3	1801	CLA	O2D-CGD-CBD	4.89	119.95	111.28
14	B4	827	CLA	O2D-CGD-CBD	4.89	119.95	111.28
14	B2	824	CLA	O2D-CGD-CBD	4.89	119.95	111.28
14	B4	806	CLA	O2D-CGD-CBD	4.89	119.95	111.28
14	B2	828	CLA	O2D-CGD-CBD	4.90	119.97	111.28
14	B1	834	CLA	O2D-CGD-CBD	4.91	119.98	111.28
14	L2	205	CLA	O2D-CGD-CBD	4.91	119.99	111.28
14	B5	1810	CLA	O2D-CGD-CBD	4.92	120.00	111.28
14	A3	845	CLA	O2D-CGD-CBD	4.92	120.00	111.28
14	B5	1835	CLA	O2D-CGD-CBD	4.93	120.02	111.28
14	B5	1816	CLA	O2D-CGD-CBD	4.94	120.05	111.28
14	B3	1810	CLA	O2D-CGD-CBD	4.95	120.06	111.28
14	B6	814	CLA	O2D-CGD-CBD	4.96	120.07	111.28
14	M6	1201	CLA	O2D-CGD-CBD	4.96	120.08	111.28
14	B3	1817	CLA	O2D-CGD-CBD	4.97	120.10	111.28
14	B6	825	CLA	O2D-CGD-CBD	4.97	120.10	111.28
14	A5	806	CLA	O2A-CGA-CBA	4.98	126.31	111.92
14	M1	1201	CLA	O2D-CGD-CBD	4.98	120.11	111.28
14	A1	805	CLA	O2A-CGA-CBA	4.98	126.32	111.92
14	A5	804	CLA	O2D-CGD-CBD	4.98	120.11	111.28
14	B1	853	CLA	O2D-CGD-CBD	4.99	120.12	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B5	1806	CLA	O2D-CGD-CBD	5.00	120.14	111.28
14	L6	206	CLA	O2D-CGD-CBD	5.00	120.14	111.28
14	A4	805	CLA	O2A-CGA-CBA	5.00	126.38	111.92
14	B1	830	CLA	O2D-CGD-CBD	5.00	120.15	111.28
14	B2	807	CLA	O2D-CGD-CBD	5.01	120.17	111.28
14	A5	843	CLA	O2D-CGD-CBD	5.02	120.18	111.28
14	B1	810	CLA	O2D-CGD-CBD	5.03	120.19	111.28
14	A2	1606	CLA	O2D-CGD-CBD	5.05	120.24	111.28
14	M2	1201	CLA	O2D-CGD-CBD	5.06	120.25	111.28
14	B1	833	CLA	O2D-CGD-CBD	5.06	120.26	111.28
14	A6	1604	CLA	O2D-CGD-CBD	5.07	120.27	111.28
14	L3	203	CLA	O2D-CGD-CBD	5.10	120.32	111.28
14	B3	1806	CLA	O2D-CGD-CBD	5.10	120.32	111.28
14	L2	202	CLA	O2D-CGD-CBD	5.13	120.37	111.28
14	B3	1831	CLA	O2D-CGD-CBD	5.13	120.37	111.28
14	B6	829	CLA	O2D-CGD-CBD	5.14	120.39	111.28
14	A4	803	CLA	O2D-CGD-CBD	5.15	120.42	111.28
14	B5	1801	CLA	O2D-CGD-CBD	5.18	120.47	111.28
14	A3	804	CLA	O2D-CGD-CBD	5.19	120.49	111.28
14	B4	810	CLA	O2D-CGD-CBD	5.23	120.55	111.28
14	A1	803	CLA	O2D-CGD-CBD	5.24	120.57	111.28
14	L1	202	CLA	O2D-CGD-CBD	5.28	120.65	111.28
14	L4	201	CLA	O2D-CGD-CBD	5.50	121.03	111.28
14	L5	203	CLA	O2D-CGD-CBD	5.57	121.15	111.28
14	A6	1633	CLA	O2D-CGD-CBD	5.58	121.17	111.28
14	B1	805	CLA	O2D-CGD-CBD	5.62	121.24	111.28
14	A3	834	CLA	O2D-CGD-CBD	5.70	121.38	111.28
14	B2	802	CLA	O2D-CGD-CBD	5.75	121.47	111.28
14	B3	1804	CLA	O2D-CGD-CBD	5.75	121.48	111.28
14	B5	1804	CLA	O2D-CGD-CBD	5.76	121.49	111.28
14	A6	1651	CLA	O2D-CGD-CBD	5.82	121.61	111.28
14	B4	804	CLA	O2D-CGD-CBD	5.87	121.68	111.28
15	A1	841	PQN	C14-C13-C15	6.35	126.24	115.29
15	A5	844	PQN	C14-C13-C15	6.49	126.49	115.29
15	A6	1642	PQN	C14-C13-C15	6.50	126.49	115.29
15	A3	846	PQN	C14-C13-C15	6.55	126.58	115.29
15	A2	1646	PQN	C14-C13-C15	6.55	126.59	115.29
15	A4	843	PQN	C14-C13-C15	6.57	126.62	115.29
14	A6	1602	CLA	O2D-CGD-CBD	9.05	127.33	111.28
14	A2	1602	CLA	O2D-CGD-CBD	9.23	127.65	111.28
14	A1	801	CLA	O2D-CGD-CBD	9.33	127.83	111.28
14	A5	801	CLA	O2D-CGD-CBD	9.37	127.88	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A4	801	CLA	O2D-CGD-CBD	9.46	128.05	111.28
14	A3	801	CLA	O2D-CGD-CBD	9.56	128.23	111.28

All (1109) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A6	1628	CLA	NA
17	A3	854	LHG	C2
14	A4	814	CLA	NC
14	A4	814	CLA	NA
14	A1	820	CLA	NC
14	A1	820	CLA	NA
14	A1	803	CLA	NC
14	A1	803	CLA	NA
14	B6	824	CLA	NC
14	B6	824	CLA	ND
14	B6	824	CLA	NA
14	B5	1825	CLA	NC
14	B5	1825	CLA	NA
14	B3	1822	CLA	NC
14	B3	1822	CLA	NA
14	B3	1802	CLA	NC
14	B3	1802	CLA	NA
14	K1	1401	CLA	NC
14	K1	1401	CLA	NA
14	B1	836	CLA	NC
14	B1	836	CLA	NA
14	A3	841	CLA	NC
14	A3	841	CLA	NA
14	B4	826	CLA	NC
14	B4	826	CLA	ND
14	B4	826	CLA	NA
14	A5	814	CLA	NC
14	A5	814	CLA	NA
14	A5	805	CLA	NA
14	A5	805	CLA	NC
14	A5	805	CLA	ND
14	A5	802	CLA	NA
14	B5	1828	CLA	NC
14	B5	1828	CLA	ND
14	B5	1828	CLA	NA
17	A6	1650	LHG	C2

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Mol	Chain	Res	Type	Atom
14	B3	1840	CLA	NC
14	B3	1840	CLA	NA
14	A6	1641	CLA	NC
14	A6	1641	CLA	ND
14	A6	1641	CLA	NA
14	B1	831	CLA	NC
14	B1	831	CLA	NA
14	L2	202	CLA	NC
14	L2	202	CLA	NA
14	B4	802	CLA	NC
14	B4	802	CLA	NA
14	B2	824	CLA	NC
14	B2	824	CLA	NA
14	A3	824	CLA	NC
14	A3	824	CLA	NA
14	A6	1640	CLA	NC
14	A6	1640	CLA	NA
14	A4	823	CLA	NC
14	A4	823	CLA	NA
14	A3	834	CLA	NC
14	A3	834	CLA	NA
14	B3	1827	CLA	NC
14	B3	1827	CLA	NA
14	J6	1103	CLA	NC
14	J6	1103	CLA	NA
14	B3	1835	CLA	NC
14	B3	1835	CLA	NA
14	B2	832	CLA	NC
14	B2	832	CLA	NA
14	A5	815	CLA	NC
14	A5	815	CLA	NA
14	A5	803	CLA	NC
14	A5	803	CLA	ND
14	A5	803	CLA	NA
14	A2	1617	CLA	NC
14	A2	1617	CLA	NA
14	B2	806	CLA	NC
14	B2	806	CLA	NA
14	A2	1605	CLA	NC
14	A2	1605	CLA	ND
14	A2	1605	CLA	NA
14	A2	1644	CLA	NC

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Mol	Chain	Res	Type	Atom
14	A2	1644	CLA	NA
14	A6	1611	CLA	NC
14	A6	1611	CLA	NA
14	B3	1829	CLA	NA
14	A2	1642	CLA	NC
14	A2	1642	CLA	NA
14	A1	825	CLA	NC
14	A1	825	CLA	NA
14	L2	206	CLA	NC
14	L2	206	CLA	NA
14	A3	843	CLA	NC
14	A3	843	CLA	NA
14	A3	811	CLA	NC
14	A3	811	CLA	NA
14	B3	1825	CLA	NC
14	B3	1825	CLA	NA
14	A6	1616	CLA	NC
14	A6	1616	CLA	NA
14	A5	820	CLA	NC
14	A5	820	CLA	NA
14	A4	842	CLA	NA
14	A4	842	CLA	NC
14	A4	842	CLA	ND
14	B6	834	CLA	NC
14	B6	834	CLA	NA
14	A2	1630	CLA	NA
14	B6	821	CLA	NC
14	B6	821	CLA	NA
14	A3	803	CLA	NC
14	A3	803	CLA	ND
14	A3	803	CLA	NA
14	A6	1619	CLA	NC
14	A6	1619	CLA	NA
14	B3	1801	CLA	NC
14	B3	1801	CLA	NA
14	B5	1834	CLA	NA
14	B5	1802	CLA	NC
14	B5	1802	CLA	NA
14	A3	837	CLA	NC
14	A3	837	CLA	ND
14	A3	837	CLA	NA
14	B5	1833	CLA	NC

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Mol	Chain	Res	Type	Atom
14	B5	1833	CLA	NA
14	A3	829	CLA	NA
14	A2	1641	CLA	NC
14	A2	1641	CLA	NA
14	B2	810	CLA	NC
14	B2	810	CLA	NA
14	A4	807	CLA	NC
14	A4	807	CLA	NA
14	F1	1301	CLA	NC
14	F1	1301	CLA	NA
14	A3	830	CLA	NC
14	A3	830	CLA	NA
14	B3	1837	CLA	NC
14	B3	1837	CLA	NA
14	B1	854	CLA	NC
14	B1	854	CLA	ND
14	B1	854	CLA	NA
14	B4	818	CLA	NC
14	B4	818	CLA	NA
14	B5	1818	CLA	NC
14	B5	1818	CLA	NA
14	B5	1836	CLA	NC
14	B5	1836	CLA	NA
14	B6	827	CLA	NA
14	B5	1807	CLA	NA
14	B5	1807	CLA	NC
14	B5	1807	CLA	ND
14	A4	815	CLA	NC
14	A4	815	CLA	NA
14	A4	840	CLA	NC
14	A4	840	CLA	NA
14	B1	830	CLA	NC
14	B1	830	CLA	NA
14	A4	833	CLA	NC
14	A4	833	CLA	NA
14	A4	812	CLA	NC
14	A4	812	CLA	ND
14	A4	812	CLA	NA
14	B3	1832	CLA	NC
14	B3	1832	CLA	NA
14	A3	818	CLA	NC
14	A3	818	CLA	NA

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Mol	Chain	Res	Type	Atom
14	A4	803	CLA	NC
14	A4	803	CLA	NA
14	A3	831	CLA	NC
14	A3	831	CLA	NA
14	B4	840	CLA	NC
14	B4	840	CLA	NA
14	A3	825	CLA	NC
14	A3	825	CLA	ND
14	A3	825	CLA	NA
14	B5	1838	CLA	NC
14	B5	1838	CLA	NA
14	B3	1818	CLA	NC
14	B3	1818	CLA	NA
14	K4	1401	CLA	NC
14	K4	1401	CLA	NA
14	L2	205	CLA	NA
14	A2	1627	CLA	NC
14	A2	1627	CLA	ND
14	A2	1627	CLA	NA
14	A1	828	CLA	NC
14	A1	828	CLA	NA
14	A5	829	CLA	NC
14	A5	829	CLA	NA
14	A1	815	CLA	NC
14	A1	815	CLA	NA
14	B1	833	CLA	NA
14	B4	829	CLA	NA
14	B1	809	CLA	NC
14	B1	809	CLA	NA
14	A4	810	CLA	NC
14	A4	810	CLA	NA
14	A1	826	CLA	NC
14	A1	826	CLA	ND
14	A1	826	CLA	NA
14	A1	840	CLA	NA
14	A1	840	CLA	NC
14	A1	840	CLA	ND
14	A4	828	CLA	NC
14	A4	828	CLA	NA
14	X1	1701	CLA	NC
14	X1	1701	CLA	NA
14	F4	202	CLA	NC

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Mol	Chain	Res	Type	Atom
14	F4	202	CLA	NA
14	A4	834	CLA	NC
14	A4	834	CLA	NA
14	B5	1810	CLA	NA
14	A3	812	CLA	NC
14	A3	812	CLA	NA
14	A1	834	CLA	NC
14	A1	834	CLA	ND
14	A1	834	CLA	NA
14	B2	830	CLA	NC
14	B2	830	CLA	NA
14	J3	102	CLA	NC
14	J3	102	CLA	NA
14	B4	815	CLA	NA
14	B4	815	CLA	NC
14	B4	815	CLA	ND
14	B6	838	CLA	NC
14	B6	838	CLA	NA
14	B2	811	CLA	NC
14	B2	811	CLA	NA
14	B5	1805	CLA	NA
14	B1	808	CLA	NC
14	B1	808	CLA	ND
14	B1	808	CLA	NA
14	L1	207	CLA	NA
14	B1	805	CLA	NA
14	B3	1810	CLA	NA
14	L6	203	CLA	NC
14	L6	203	CLA	NA
14	J4	102	CLA	NC
14	J4	102	CLA	NA
14	B4	831	CLA	NC
14	B4	831	CLA	NA
14	B3	1824	CLA	NC
14	B3	1824	CLA	NA
14	A6	1618	CLA	NC
14	A6	1618	CLA	NA
14	A2	1637	CLA	NC
14	A2	1637	CLA	NA
14	B5	1821	CLA	NC
14	B5	1821	CLA	NA
14	L2	207	CLA	NC

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Mol	Chain	Res	Type	Atom
14	L2	207	CLA	NA
14	A2	1607	CLA	NA
14	A2	1607	CLA	NC
14	A2	1607	CLA	ND
14	A6	1606	CLA	NC
14	A6	1606	CLA	ND
14	A6	1606	CLA	NA
14	L5	202	CLA	NC
14	L5	202	CLA	NA
14	B1	840	CLA	NA
14	B2	828	CLA	NC
14	B2	828	CLA	NA
14	B4	832	CLA	NC
14	B4	832	CLA	NA
14	B6	811	CLA	NC
14	B6	811	CLA	NA
14	B3	1815	CLA	NA
14	B3	1815	CLA	NC
14	B3	1815	CLA	ND
14	A3	808	CLA	NC
14	A3	808	CLA	NA
14	B2	812	CLA	NA
14	B2	812	CLA	NC
14	B2	812	CLA	ND
14	K3	1401	CLA	NC
14	K3	1401	CLA	NA
14	A2	1632	CLA	NC
14	A2	1632	CLA	NA
14	B2	823	CLA	NC
14	B2	823	CLA	ND
14	B2	823	CLA	NA
14	A4	805	CLA	NC
14	A4	805	CLA	ND
14	A4	805	CLA	NA
14	A4	836	CLA	NA
14	A5	813	CLA	NC
14	A5	813	CLA	ND
14	A5	813	CLA	NA
14	B1	819	CLA	NA
14	B3	1816	CLA	NC
14	B3	1816	CLA	NA
14	B3	1813	CLA	NC

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Mol	Chain	Res	Type	Atom
14	B3	1813	CLA	NA
14	A5	809	CLA	NC
14	A5	809	CLA	NA
14	A4	826	CLA	NC
14	A4	826	CLA	ND
14	A4	826	CLA	NA
14	A5	836	CLA	NC
14	A5	836	CLA	ND
14	A5	836	CLA	NA
14	A1	805	CLA	NC
14	A1	805	CLA	ND
14	A1	805	CLA	NA
14	B6	828	CLA	NA
14	A3	804	CLA	NC
14	A3	804	CLA	NA
14	B3	1803	CLA	NA
14	B2	803	CLA	NA
14	A2	1625	CLA	NA
14	B4	810	CLA	NA
14	A2	1610	CLA	NC
14	A2	1610	CLA	NA
14	B1	826	CLA	NC
14	B1	826	CLA	NA
14	A1	833	CLA	NC
14	A1	833	CLA	NA
14	A6	1638	CLA	NA
14	B2	816	CLA	NA
14	B1	823	CLA	NC
14	B1	823	CLA	NA
14	L4	203	CLA	NA
14	B4	838	CLA	NC
14	B4	838	CLA	NA
14	B1	821	CLA	NC
14	B1	821	CLA	NA
14	A6	1637	CLA	NA
14	A6	1617	CLA	NC
14	A6	1617	CLA	NA
14	A3	820	CLA	NC
14	A3	820	CLA	NA
14	A1	809	CLA	NA
14	A3	827	CLA	NC
14	A3	827	CLA	ND

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Mol	Chain	Res	Type	Atom
14	A3	827	CLA	NA
14	A2	1611	CLA	NC
14	A2	1611	CLA	NA
14	B6	835	CLA	NC
14	B6	835	CLA	NA
14	A5	828	CLA	NA
14	A1	814	CLA	NC
14	A1	814	CLA	NA
14	B1	825	CLA	NC
14	B1	825	CLA	ND
14	B1	825	CLA	NA
14	B3	1833	CLA	NC
14	B3	1833	CLA	NA
14	B6	818	CLA	NC
14	B6	818	CLA	NA
17	A1	849	LHG	C2
14	B3	1830	CLA	NA
14	A6	1624	CLA	NC
14	A6	1624	CLA	NA
14	L6	202	CLA	NC
14	L6	202	CLA	NA
14	A2	1616	CLA	NC
14	A2	1616	CLA	NA
14	A3	815	CLA	NC
14	A3	815	CLA	NA
14	A1	823	CLA	NC
14	A1	823	CLA	NA
14	B5	1806	CLA	NA
14	A1	808	CLA	NC
14	A1	808	CLA	NA
14	B6	829	CLA	NC
14	B6	829	CLA	NA
14	A1	817	CLA	NA
14	A5	834	CLA	NC
14	A5	834	CLA	NA
14	B2	825	CLA	NC
14	B2	825	CLA	ND
14	B2	825	CLA	NA
14	B3	1809	CLA	NC
14	B3	1809	CLA	NA
14	A5	821	CLA	NC
14	A5	821	CLA	NA

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Mol	Chain	Res	Type	Atom
14	B1	853	CLA	NC
14	B1	853	CLA	NA
14	A2	1620	CLA	NA
14	A5	841	CLA	NC
14	A5	841	CLA	NA
14	X4	102	CLA	NC
14	X4	102	CLA	NA
14	B6	802	CLA	NA
14	B3	1843	CLA	NC
14	B3	1843	CLA	NA
14	A5	816	CLA	NC
14	A5	816	CLA	NA
14	M1	1201	CLA	NA
14	B3	1838	CLA	NC
14	B3	1838	CLA	NA
14	B6	806	CLA	NA
14	B6	806	CLA	NC
14	B6	806	CLA	ND
14	A4	819	CLA	NC
14	A4	819	CLA	NA
14	B5	1823	CLA	NC
14	B5	1823	CLA	NA
14	B6	810	CLA	NC
14	B6	810	CLA	ND
14	B6	810	CLA	NA
14	A3	832	CLA	NC
14	A3	832	CLA	NA
14	A4	813	CLA	NC
14	A4	813	CLA	NA
14	A5	842	CLA	NC
14	A5	842	CLA	NA
14	A6	1607	CLA	NA
14	B2	819	CLA	NC
14	B2	819	CLA	NA
14	B4	820	CLA	NA
14	A1	810	CLA	NC
14	A1	810	CLA	NA
14	L4	205	CLA	NC
14	L4	205	CLA	NA
14	B5	1830	CLA	NA
14	A6	1601	CLA	NC
14	A6	1601	CLA	NA

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Mol	Chain	Res	Type	Atom
14	A6	1626	CLA	NC
14	A6	1626	CLA	NA
14	B2	813	CLA	NC
14	B2	813	CLA	NA
14	B2	837	CLA	NC
14	B2	837	CLA	NA
14	B6	841	CLA	NC
14	B6	841	CLA	NA
14	A3	844	CLA	NC
14	A3	844	CLA	ND
14	A3	844	CLA	NA
14	B6	825	CLA	NC
14	B6	825	CLA	NA
14	F5	1301	CLA	NC
14	F5	1301	CLA	NA
14	B3	1812	CLA	NC
14	B3	1812	CLA	ND
14	B3	1812	CLA	NA
14	F6	202	CLA	NC
14	F6	202	CLA	NA
14	B6	837	CLA	NC
14	B6	837	CLA	ND
14	B6	837	CLA	NA
14	A1	827	CLA	NA
14	A4	824	CLA	NC
14	A4	824	CLA	ND
14	A4	824	CLA	NA
14	B2	829	CLA	NC
14	B2	829	CLA	NA
14	L5	205	CLA	NC
14	L5	205	CLA	NA
14	A5	801	CLA	NA
14	A2	1634	CLA	NC
14	A2	1634	CLA	NA
14	A4	838	CLA	NC
14	A4	838	CLA	NA
14	B6	836	CLA	NC
14	B6	836	CLA	NA
14	A1	824	CLA	NC
14	A1	824	CLA	ND
14	A1	824	CLA	NA
14	B5	1820	CLA	NC

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Mol	Chain	Res	Type	Atom
14	B5	1820	CLA	NA
14	B5	1842	CLA	NC
14	B5	1842	CLA	NA
14	A1	839	CLA	NC
14	A1	839	CLA	NA
14	A5	808	CLA	NC
14	A5	808	CLA	NA
14	A4	816	CLA	NC
14	A4	816	CLA	NA
14	B1	839	CLA	NA
14	A6	1623	CLA	NA
14	A6	1603	CLA	NC
14	A6	1603	CLA	NA
14	B5	1812	CLA	NC
14	B5	1812	CLA	ND
14	B5	1812	CLA	NA
14	A6	1636	CLA	NC
14	A6	1636	CLA	ND
14	A6	1636	CLA	NA
14	B3	1817	CLA	NC
14	A5	839	CLA	NC
14	A5	839	CLA	NA
14	B4	823	CLA	NC
14	B4	823	CLA	NA
14	A2	1638	CLA	NC
14	A2	1638	CLA	ND
14	A2	1638	CLA	NA
14	B4	852	CLA	NC
14	B4	852	CLA	NA
14	L5	204	CLA	NC
14	L5	204	CLA	NA
14	L3	202	CLA	NC
14	L3	202	CLA	NA
14	A4	853	CLA	NC
14	A4	853	CLA	NA
14	B4	806	CLA	NA
14	A5	835	CLA	NC
14	A5	835	CLA	NA
14	A5	840	CLA	NC
14	A5	840	CLA	NA
14	B2	805	CLA	NC
14	B2	805	CLA	ND

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Mol	Chain	Res	Type	Atom
14	B2	805	CLA	NA
14	A2	1631	CLA	NC
14	A2	1631	CLA	NA
14	B5	1839	CLA	NC
14	B5	1839	CLA	ND
14	B5	1839	CLA	NA
14	A2	1623	CLA	NC
14	A2	1623	CLA	NA
14	B3	1819	CLA	NC
14	B3	1819	CLA	NA
14	B4	808	CLA	NC
14	B4	808	CLA	ND
14	B4	808	CLA	NA
14	A5	825	CLA	NC
14	A5	825	CLA	ND
14	A5	825	CLA	NA
14	L6	207	CLA	NC
14	L6	207	CLA	NA
14	B2	839	CLA	NC
14	B2	839	CLA	NA
14	B3	1808	CLA	NC
14	B3	1808	CLA	ND
14	B3	1808	CLA	NA
14	A6	1610	CLA	NA
14	L1	206	CLA	NC
14	L1	206	CLA	NA
14	A2	1643	CLA	NC
14	A2	1643	CLA	NA
14	A4	804	CLA	NA
14	A4	804	CLA	NC
14	A4	804	CLA	ND
14	B6	808	CLA	NA
14	B1	837	CLA	NC
14	B1	837	CLA	NA
14	A1	829	CLA	NC
14	A1	829	CLA	NA
14	A4	809	CLA	NA
14	J6	1102	CLA	NC
14	J6	1102	CLA	ND
14	J6	1102	CLA	NA
14	A2	1639	CLA	NA
14	B6	832	CLA	NA

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Mol	Chain	Res	Type	Atom
14	A1	837	CLA	NC
14	A1	837	CLA	NA
14	A4	841	CLA	NC
14	A4	841	CLA	NA
14	F2	202	CLA	NC
14	F2	202	CLA	NA
14	A3	816	CLA	NC
14	A3	816	CLA	NA
14	A3	817	CLA	NC
14	A3	817	CLA	NA
14	B3	1826	CLA	NC
14	B3	1826	CLA	ND
14	B3	1826	CLA	NA
14	A2	1636	CLA	NC
14	A2	1636	CLA	NA
14	B3	1814	CLA	NC
14	B3	1814	CLA	NA
14	B4	824	CLA	NC
14	B4	824	CLA	NA
14	B3	1820	CLA	NA
14	A6	1605	CLA	NA
14	A6	1605	CLA	NC
14	A6	1605	CLA	ND
14	A5	806	CLA	NC
14	A5	806	CLA	ND
14	A5	806	CLA	NA
14	A6	1630	CLA	NC
14	A6	1630	CLA	NA
14	B4	830	CLA	NA
14	A3	845	CLA	NC
14	A3	845	CLA	NA
14	A2	1609	CLA	NC
14	A2	1609	CLA	NA
14	B4	819	CLA	NC
14	B4	819	CLA	NA
14	B5	1841	CLA	NA
14	B4	816	CLA	NC
14	B4	816	CLA	NA
14	B6	817	CLA	NC
14	B6	817	CLA	NA
14	B4	841	CLA	NA
14	A3	813	CLA	NC

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Mol	Chain	Res	Type	Atom
14	A3	813	CLA	ND
14	A3	813	CLA	NA
14	B4	822	CLA	NC
14	B4	822	CLA	NA
14	B4	828	CLA	NC
14	B4	828	CLA	ND
14	B4	828	CLA	NA
14	B1	820	CLA	NC
14	B1	820	CLA	NA
14	B1	835	CLA	NC
14	B1	835	CLA	NA
14	B6	839	CLA	NA
14	L3	203	CLA	NC
14	L3	203	CLA	NA
14	A5	812	CLA	NC
14	A5	812	CLA	NA
14	B2	801	CLA	NA
14	B1	827	CLA	NC
14	B1	827	CLA	ND
14	B1	827	CLA	NA
14	A2	1606	CLA	NC
14	A2	1606	CLA	NA
14	A2	1615	CLA	NC
14	A2	1615	CLA	ND
14	A2	1615	CLA	NA
14	A5	838	CLA	NA
14	B1	828	CLA	NA
14	B6	819	CLA	NC
14	B6	819	CLA	NA
14	B3	1842	CLA	NC
14	B3	1842	CLA	NA
14	K6	1401	CLA	NC
14	K6	1401	CLA	NA
14	A5	804	CLA	NC
14	A5	804	CLA	NA
14	X6	1701	CLA	NC
14	X6	1701	CLA	NA
14	L1	205	CLA	NA
14	B4	807	CLA	NA
14	B4	807	CLA	NC
14	B4	807	CLA	ND
14	B1	838	CLA	NC

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Mol	Chain	Res	Type	Atom
14	B1	838	CLA	ND
14	B1	838	CLA	NA
14	B4	825	CLA	NC
14	B4	825	CLA	NA
14	A6	1613	CLA	NC
14	A6	1613	CLA	ND
14	A6	1613	CLA	NA
14	A3	809	CLA	NC
14	A3	809	CLA	NA
14	A6	1622	CLA	NC
14	A6	1622	CLA	NA
14	A2	1612	CLA	NA
14	B1	812	CLA	NC
14	B1	812	CLA	NA
17	A2	1654	LHG	C2
14	A5	819	CLA	NC
14	A5	819	CLA	NA
14	B6	830	CLA	NC
14	B6	830	CLA	NA
14	B5	1835	CLA	NC
14	B5	1835	CLA	NA
14	A2	1629	CLA	NC
14	A2	1629	CLA	ND
14	A2	1629	CLA	NA
14	J5	101	CLA	NC
14	J5	101	CLA	ND
14	J5	101	CLA	NA
14	A6	1621	CLA	NC
14	A6	1621	CLA	NA
14	X3	102	CLA	NC
14	X3	102	CLA	NA
14	L1	202	CLA	NC
14	L1	202	CLA	NA
14	B1	841	CLA	NC
14	B1	841	CLA	NA
14	A2	1626	CLA	NC
14	A2	1626	CLA	NA
14	A3	842	CLA	NC
14	A3	842	CLA	NA
14	A1	801	CLA	NA
14	A3	822	CLA	NC
14	A3	822	CLA	NA

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Mol	Chain	Res	Type	Atom
14	L6	208	CLA	NA
14	A4	802	CLA	NC
14	A4	802	CLA	ND
14	A4	802	CLA	NA
14	B4	804	CLA	NA
14	A5	817	CLA	NC
14	A5	817	CLA	NA
14	A1	807	CLA	NC
14	A1	807	CLA	NA
14	B2	814	CLA	NC
14	B2	814	CLA	NA
14	A2	1604	CLA	NC
14	A2	1604	CLA	NA
14	A1	802	CLA	NC
14	A1	802	CLA	ND
14	A1	802	CLA	NA
14	B2	836	CLA	NC
14	B2	836	CLA	ND
14	B2	836	CLA	NA
14	A6	1635	CLA	NC
14	A6	1635	CLA	NA
14	B2	817	CLA	NC
14	B2	817	CLA	NA
14	B5	1819	CLA	NC
14	B5	1819	CLA	NA
14	L1	201	CLA	NC
14	L1	201	CLA	NA
14	A6	1629	CLA	NC
14	A6	1629	CLA	NA
14	A1	835	CLA	NA
14	B3	1805	CLA	NA
14	B3	1821	CLA	NC
14	B3	1821	CLA	NA
14	M6	1201	CLA	NA
14	B4	827	CLA	NC
14	B4	827	CLA	NA
14	B5	1803	CLA	NA
14	A4	811	CLA	NC
14	A4	811	CLA	NA
14	A1	804	CLA	NA
14	A1	804	CLA	NC
14	A1	804	CLA	ND

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Mol	Chain	Res	Type	Atom
14	B2	834	CLA	NC
14	B2	834	CLA	NA
14	B3	1836	CLA	NC
14	B3	1836	CLA	NA
14	B4	803	CLA	NA
14	A2	1633	CLA	NC
14	A2	1633	CLA	NA
14	A2	1613	CLA	NC
14	A2	1613	CLA	NA
14	A4	817	CLA	NA
14	A3	836	CLA	NC
14	A3	836	CLA	NA
14	A4	808	CLA	NC
14	A4	808	CLA	NA
14	B2	804	CLA	NA
14	B2	804	CLA	NC
14	B2	804	CLA	ND
14	A6	1614	CLA	NC
14	A6	1614	CLA	NA
14	B4	813	CLA	NC
14	B4	813	CLA	NA
14	B1	813	CLA	NC
14	B1	813	CLA	NA
14	B2	820	CLA	NC
14	B2	820	CLA	NA
14	B5	1837	CLA	NC
14	B5	1837	CLA	NA
14	A2	1622	CLA	NC
14	A2	1622	CLA	NA
14	A5	807	CLA	NC
14	A5	807	CLA	NA
14	A1	821	CLA	NC
14	A1	821	CLA	NA
14	A2	1621	CLA	NC
14	A2	1621	CLA	NA
14	A1	836	CLA	NA
14	B1	817	CLA	NC
14	B1	817	CLA	NA
14	B6	840	CLA	NC
14	B6	840	CLA	NA
14	A4	801	CLA	NA
14	A5	823	CLA	NA

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Mol	Chain	Res	Type	Atom
14	B5	1840	CLA	NC
14	B5	1840	CLA	NA
14	J1	102	CLA	NC
14	J1	102	CLA	NA
14	A3	814	CLA	NC
14	A3	814	CLA	NA
14	B3	1804	CLA	NA
14	A5	811	CLA	NC
14	A5	811	CLA	NA
14	X2	1701	CLA	NC
14	X2	1701	CLA	NA
14	A1	812	CLA	NC
14	A1	812	CLA	ND
14	A1	812	CLA	NA
14	B6	822	CLA	NC
14	B6	822	CLA	NA
14	J4	101	CLA	NC
14	J4	101	CLA	ND
14	J4	101	CLA	NA
14	B6	813	CLA	NA
14	B6	813	CLA	NC
14	B6	813	CLA	ND
14	B1	802	CLA	NC
14	B1	802	CLA	NA
14	B1	815	CLA	NC
14	B1	815	CLA	NA
14	J3	101	CLA	NC
14	J3	101	CLA	ND
14	J3	101	CLA	NA
14	F2	204	CLA	NC
14	F2	204	CLA	NA
14	B4	839	CLA	NC
14	B4	839	CLA	ND
14	B4	839	CLA	NA
14	B4	833	CLA	NC
14	B4	833	CLA	NA
14	A4	827	CLA	NA
14	J6	1101	CLA	NC
14	J6	1101	CLA	ND
14	J6	1101	CLA	NA
14	K2	1401	CLA	NC
14	K2	1401	CLA	NA

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Mol	Chain	Res	Type	Atom
14	B3	1807	CLA	NA
14	B3	1807	CLA	NC
14	B3	1807	CLA	ND
14	A2	1628	CLA	NC
14	A2	1628	CLA	NA
14	A3	807	CLA	NC
14	A3	807	CLA	NA
14	A3	810	CLA	NA
14	B3	1834	CLA	NA
14	A2	1608	CLA	NC
14	A2	1608	CLA	ND
14	A2	1608	CLA	NA
14	B4	843	CLA	NC
14	B4	843	CLA	NA
14	A6	1604	CLA	NC
14	A6	1604	CLA	NA
14	B5	1824	CLA	NC
14	B5	1824	CLA	NA
14	B3	1806	CLA	NA
14	B5	1843	CLA	NC
14	B5	1843	CLA	NA
14	B2	818	CLA	NC
14	B2	818	CLA	NA
14	A6	1609	CLA	NC
14	A6	1609	CLA	NA
14	B5	1826	CLA	NC
14	B5	1826	CLA	ND
14	B5	1826	CLA	NA
14	K5	101	CLA	NA
14	K5	101	CLA	NC
14	K5	101	CLA	ND
14	A1	818	CLA	NC
14	A1	818	CLA	NA
14	A5	810	CLA	NA
14	F3	202	CLA	NC
14	F3	202	CLA	NA
14	A3	806	CLA	NC
14	A3	806	CLA	ND
14	A3	806	CLA	NA
14	A1	816	CLA	NC
14	A1	816	CLA	NA
14	B6	805	CLA	NA

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Mol	Chain	Res	Type	Atom
14	B6	804	CLA	NA
14	B4	834	CLA	NA
14	A3	826	CLA	NC
14	A3	826	CLA	NA
14	A3	840	CLA	NC
14	A3	840	CLA	NA
14	B2	835	CLA	NC
14	B2	835	CLA	NA
14	B2	807	CLA	NA
14	A2	1618	CLA	NC
14	A2	1618	CLA	NA
14	B2	802	CLA	NA
14	B2	833	CLA	NC
14	B2	833	CLA	NA
14	M2	1201	CLA	NA
14	A3	821	CLA	NC
14	A3	821	CLA	NA
14	B3	1831	CLA	NC
14	B3	1831	CLA	NA
14	A1	838	CLA	NC
14	A1	838	CLA	NA
14	B6	820	CLA	NC
14	B6	820	CLA	NA
14	B4	809	CLA	NC
14	B4	809	CLA	NA
14	B4	837	CLA	NC
14	B4	837	CLA	NA
14	A2	1640	CLA	NA
14	A3	805	CLA	NA
14	A3	805	CLA	NC
14	A3	805	CLA	ND
14	B3	1839	CLA	NC
14	B3	1839	CLA	ND
14	B3	1839	CLA	NA
14	A5	827	CLA	NC
14	A5	827	CLA	ND
14	A5	827	CLA	NA
14	A5	831	CLA	NC
14	A5	831	CLA	NA
14	A4	822	CLA	NA
14	A6	1631	CLA	NC
14	A6	1631	CLA	NA

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Mol	Chain	Res	Type	Atom
14	B2	831	CLA	NA
14	A4	818	CLA	NC
14	A4	818	CLA	NA
14	B4	842	CLA	NC
14	B4	842	CLA	NA
14	B5	1829	CLA	NA
14	B5	1832	CLA	NC
14	B5	1832	CLA	NA
14	A6	1615	CLA	NC
14	A6	1615	CLA	NA
14	A4	820	CLA	NC
14	A4	820	CLA	NA
14	B4	805	CLA	NA
14	B1	814	CLA	NA
14	B1	814	CLA	NC
14	B1	814	CLA	ND
14	B2	821	CLA	NC
14	B2	821	CLA	NA
14	A1	811	CLA	NC
14	A1	811	CLA	NA
14	B1	832	CLA	NC
14	B1	832	CLA	NA
14	B5	1804	CLA	NA
14	B1	818	CLA	NC
14	B1	818	CLA	NA
14	B5	1827	CLA	NC
14	B5	1827	CLA	NA
14	A4	829	CLA	NC
14	A4	829	CLA	NA
14	B2	809	CLA	NC
14	B2	809	CLA	ND
14	B2	809	CLA	NA
14	L4	201	CLA	NC
14	L4	201	CLA	NA
14	A5	837	CLA	NA
14	A3	823	CLA	NA
14	B4	812	CLA	NC
14	B4	812	CLA	ND
14	B4	812	CLA	NA
14	I1	101	CLA	NC
14	I1	101	CLA	NA
14	B1	824	CLA	NC

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Mol	Chain	Res	Type	Atom
14	B1	824	CLA	NA
14	A5	824	CLA	NC
14	A5	824	CLA	NA
14	A6	1634	CLA	NC
14	A6	1634	CLA	NA
14	B1	807	CLA	NA
14	B1	807	CLA	NC
14	B1	807	CLA	ND
14	B4	814	CLA	NC
14	B4	814	CLA	NA
14	B2	827	CLA	NA
14	B3	1828	CLA	NC
14	B3	1828	CLA	ND
14	B3	1828	CLA	NA
17	A5	852	LHG	C2
14	A6	1612	CLA	NC
14	A6	1612	CLA	NA
14	A5	832	CLA	NC
14	A5	832	CLA	NA
14	B1	810	CLA	NA
14	A1	813	CLA	NC
14	A1	813	CLA	NA
14	A1	819	CLA	NC
14	A1	819	CLA	NA
14	L6	206	CLA	NC
14	L6	206	CLA	NA
14	L5	206	CLA	NA
14	B1	834	CLA	NC
14	B1	834	CLA	NA
14	L4	204	CLA	NC
14	L4	204	CLA	NA
14	B5	1814	CLA	NC
14	B5	1814	CLA	NA
14	B4	817	CLA	NC
14	B4	817	CLA	NA
14	A6	1627	CLA	NC
14	A6	1627	CLA	ND
14	A6	1627	CLA	NA
14	J1	101	CLA	NC
14	J1	101	CLA	ND
14	J1	101	CLA	NA
14	A5	826	CLA	NC

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Mol	Chain	Res	Type	Atom
14	A5	826	CLA	NA
14	A2	1619	CLA	NC
14	A2	1619	CLA	NA
14	A4	835	CLA	NC
14	A4	835	CLA	ND
14	A4	835	CLA	NA
14	A3	839	CLA	NA
14	A4	830	CLA	NC
14	A4	830	CLA	NA
14	A6	1608	CLA	NC
14	A6	1608	CLA	NA
17	A4	851	LHG	C2
14	L5	203	CLA	NC
14	L5	203	CLA	NA
14	A5	830	CLA	NC
14	A5	830	CLA	NA
14	B3	1841	CLA	NA
14	A2	1645	CLA	NA
14	A2	1645	CLA	NC
14	A2	1645	CLA	ND
14	B5	1813	CLA	NC
14	B5	1813	CLA	NA
14	A2	1603	CLA	NA
14	A3	828	CLA	NA
14	A2	1614	CLA	NC
14	A2	1614	CLA	NA
14	B1	822	CLA	NC
14	B1	822	CLA	NA
14	B5	1809	CLA	NC
14	B5	1809	CLA	NA
14	J5	102	CLA	NC
14	J5	102	CLA	NA
14	A3	835	CLA	NC
14	A3	835	CLA	NA
14	A4	831	CLA	NC
14	A4	831	CLA	NA
14	B3	1823	CLA	NC
14	B3	1823	CLA	NA
14	A2	1624	CLA	NC
14	A2	1624	CLA	NA
14	B1	829	CLA	NA
14	L3	205	CLA	NA

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Mol	Chain	Res	Type	Atom
14	K5	102	CLA	NC
14	K5	102	CLA	NA
14	B6	807	CLA	NC
14	B6	807	CLA	ND
14	B6	807	CLA	NA
14	B2	840	CLA	NC
14	B2	840	CLA	NA
14	B2	815	CLA	NC
14	B2	815	CLA	NA
14	B6	823	CLA	NC
14	B6	823	CLA	NA
14	A5	843	CLA	NC
14	A5	843	CLA	NA
14	B4	801	CLA	NA
14	B5	1815	CLA	NA
14	B5	1815	CLA	NC
14	B5	1815	CLA	ND
14	A1	822	CLA	NA
14	A5	822	CLA	NC
14	A5	822	CLA	NA
14	A4	821	CLA	NC
14	A4	821	CLA	NA
14	A3	838	CLA	NA
14	B4	836	CLA	NC
14	B4	836	CLA	NA
14	B1	804	CLA	NA
14	J2	101	CLA	NC
14	J2	101	CLA	ND
14	J2	101	CLA	NA
14	B1	816	CLA	NA
14	B2	822	CLA	NC
14	B2	822	CLA	NA
14	B6	814	CLA	NC
14	B6	814	CLA	NA
14	B6	831	CLA	NC
14	B6	831	CLA	NA
14	B2	838	CLA	NA
14	B6	803	CLA	NC
14	B6	803	CLA	NA
14	A6	1625	CLA	NC
14	A6	1625	CLA	ND
14	A6	1625	CLA	NA

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Mol	Chain	Res	Type	Atom
14	A6	1651	CLA	NA
14	B5	1801	CLA	NC
14	B5	1801	CLA	NA
14	A2	1601	CLA	NC
14	A2	1601	CLA	NA
14	B5	1822	CLA	NC
14	B5	1822	CLA	NA
14	B6	826	CLA	NC
14	B6	826	CLA	ND
14	B6	826	CLA	NA
14	B5	1817	CLA	NC
14	B5	1817	CLA	NA
14	B1	806	CLA	NA
14	I6	101	CLA	NA
14	A1	806	CLA	NC
14	A1	806	CLA	NA
14	A1	832	CLA	NC
14	A1	832	CLA	NA
14	B1	801	CLA	NA
14	B2	826	CLA	NA
14	A1	830	CLA	NC
14	A1	830	CLA	NA
14	A4	825	CLA	NC
14	A4	825	CLA	NA
14	A6	1633	CLA	NC
14	A6	1633	CLA	NA
14	L3	204	CLA	NC
14	L3	204	CLA	NA
14	B5	1831	CLA	NC
14	B5	1831	CLA	NA
14	A6	1639	CLA	NC
14	A6	1639	CLA	NA
14	B6	815	CLA	NC
14	B6	812	CLA	NC
14	B6	812	CLA	NA
14	A5	818	CLA	NA
14	A4	806	CLA	NC
14	A4	806	CLA	NA
14	B4	821	CLA	NC
14	B4	821	CLA	NA
14	X5	101	CLA	NC
14	X5	101	CLA	NA

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Mol	Chain	Res	Type	Atom
14	A3	802	CLA	NA
14	A4	839	CLA	NC
14	A4	839	CLA	NA
14	B1	803	CLA	NC
14	B1	803	CLA	NA
14	A2	1602	CLA	NA
14	A6	1620	CLA	NC
14	A6	1620	CLA	NA
14	B4	835	CLA	NC
14	B4	835	CLA	NA
14	A3	819	CLA	NC
14	A3	819	CLA	NA
14	B5	1808	CLA	NC
14	B5	1808	CLA	ND
14	B5	1808	CLA	NA
14	M3	1601	CLA	NC
14	M3	1601	CLA	NA
14	B6	816	CLA	NC
14	B6	816	CLA	NA
14	B6	833	CLA	NC
14	B6	833	CLA	NA
14	B5	1816	CLA	NC
14	B5	1816	CLA	NA

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A3	816	CLA	CED-O2D-CGD-CBD
14	A1	815	CLA	CED-O2D-CGD-CBD
14	A4	815	CLA	CED-O2D-CGD-CBD
14	A6	1616	CLA	CED-O2D-CGD-CBD
14	A2	1618	CLA	CED-O2D-CGD-CBD
14	A5	816	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

743 monomers are involved in 3480 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A1	801	CLA	10	0
14	A1	802	CLA	2	0
14	A1	803	CLA	4	0
14	A1	804	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A1	805	CLA	4	0
14	A1	806	CLA	2	0
14	A1	807	CLA	5	0
14	A1	808	CLA	2	0
14	A1	809	CLA	2	0
14	A1	810	CLA	8	0
14	A1	811	CLA	2	0
14	A1	812	CLA	3	0
14	A1	813	CLA	5	0
14	A1	814	CLA	3	0
14	A1	815	CLA	1	0
14	A1	816	CLA	3	0
14	A1	817	CLA	9	0
14	A1	818	CLA	6	0
14	A1	819	CLA	1	0
14	A1	820	CLA	6	0
14	A1	821	CLA	3	0
14	A1	822	CLA	2	0
14	A1	824	CLA	5	0
14	A1	825	CLA	8	0
14	A1	826	CLA	3	0
14	A1	827	CLA	10	0
14	A1	828	CLA	4	0
14	A1	829	CLA	9	0
14	A1	830	CLA	5	0
14	A1	831	CLA	1	0
14	A1	832	CLA	4	0
14	A1	833	CLA	2	0
14	A1	834	CLA	4	0
14	A1	835	CLA	4	0
14	A1	836	CLA	4	0
14	A1	837	CLA	2	0
14	A1	838	CLA	3	0
14	A1	839	CLA	8	0
14	A1	840	CLA	3	0
15	A1	841	PQN	3	0
16	A1	842	BCR	3	0
16	A1	843	BCR	5	0
16	A1	844	BCR	2	0
16	A1	845	BCR	2	0
16	A1	846	BCR	3	0
16	A1	847	BCR	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A1	848	LHG	3	0
17	A1	849	LHG	3	0
18	A1	850	SF4	6	0
14	A2	1601	CLA	6	0
14	A2	1602	CLA	10	0
14	A2	1603	CLA	4	0
14	A2	1604	CLA	9	0
14	A2	1605	CLA	1	0
14	A2	1606	CLA	3	0
14	A2	1607	CLA	8	0
14	A2	1608	CLA	4	0
14	A2	1609	CLA	4	0
14	A2	1610	CLA	6	0
14	A2	1611	CLA	4	0
14	A2	1612	CLA	2	0
14	A2	1613	CLA	6	0
14	A2	1614	CLA	1	0
14	A2	1615	CLA	7	0
14	A2	1616	CLA	5	0
14	A2	1617	CLA	1	0
14	A2	1618	CLA	3	0
14	A2	1619	CLA	3	0
14	A2	1620	CLA	6	0
14	A2	1621	CLA	5	0
14	A2	1622	CLA	2	0
14	A2	1623	CLA	12	0
14	A2	1624	CLA	3	0
14	A2	1625	CLA	2	0
14	A2	1626	CLA	1	0
14	A2	1627	CLA	9	0
14	A2	1628	CLA	4	0
14	A2	1629	CLA	3	0
14	A2	1630	CLA	11	0
14	A2	1631	CLA	8	0
14	A2	1632	CLA	5	0
14	A2	1633	CLA	8	0
14	A2	1634	CLA	5	0
14	A2	1635	CLA	1	0
14	A2	1636	CLA	4	0
14	A2	1637	CLA	2	0
14	A2	1638	CLA	2	0
14	A2	1639	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A2	1640	CLA	2	0
14	A2	1641	CLA	2	0
14	A2	1642	CLA	2	0
14	A2	1643	CLA	4	0
14	A2	1644	CLA	9	0
15	A2	1646	PQN	3	0
16	A2	1647	BCR	2	0
16	A2	1648	BCR	2	0
16	A2	1649	BCR	1	0
16	A2	1650	BCR	3	0
16	A2	1651	BCR	3	0
16	A2	1652	BCR	10	0
17	A2	1653	LHG	2	0
17	A2	1654	LHG	3	0
18	A2	1655	SF4	4	0
14	A3	801	CLA	10	0
14	A3	802	CLA	5	0
14	A3	803	CLA	2	0
14	A3	804	CLA	3	0
14	A3	805	CLA	11	0
14	A3	806	CLA	4	0
14	A3	807	CLA	2	0
14	A3	808	CLA	7	0
14	A3	809	CLA	3	0
14	A3	810	CLA	1	0
14	A3	811	CLA	9	0
14	A3	814	CLA	5	0
14	A3	815	CLA	1	0
14	A3	816	CLA	2	0
14	A3	817	CLA	3	0
14	A3	818	CLA	8	0
14	A3	819	CLA	8	0
14	A3	820	CLA	2	0
14	A3	821	CLA	8	0
14	A3	822	CLA	4	0
14	A3	823	CLA	1	0
14	A3	824	CLA	1	0
14	A3	825	CLA	10	0
14	A3	826	CLA	4	0
14	A3	827	CLA	3	0
14	A3	828	CLA	11	0
14	A3	829	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A3	830	CLA	7	0
14	A3	831	CLA	3	0
14	A3	832	CLA	3	0
14	A3	833	CLA	1	0
14	A3	834	CLA	13	0
14	A3	835	CLA	3	0
14	A3	836	CLA	1	0
14	A3	837	CLA	5	0
14	A3	838	CLA	4	0
14	A3	839	CLA	6	0
14	A3	840	CLA	2	0
14	A3	841	CLA	2	0
14	A3	842	CLA	6	0
14	A3	843	CLA	10	0
14	A3	844	CLA	2	0
14	A3	845	CLA	4	0
15	A3	846	PQN	2	0
16	A3	847	BCR	3	0
16	A3	848	BCR	2	0
16	A3	849	BCR	2	0
16	A3	850	BCR	2	0
16	A3	851	BCR	3	0
16	A3	852	BCR	14	0
17	A3	853	LHG	2	0
17	A3	854	LHG	3	0
18	A3	855	SF4	8	0
16	A3	856	BCR	2	0
14	A4	801	CLA	12	0
14	A4	802	CLA	1	0
14	A4	803	CLA	4	0
14	A4	804	CLA	8	0
14	A4	805	CLA	4	0
14	A4	806	CLA	5	0
14	A4	807	CLA	6	0
14	A4	808	CLA	2	0
14	A4	809	CLA	1	0
14	A4	810	CLA	6	0
14	A4	811	CLA	1	0
14	A4	812	CLA	1	0
14	A4	813	CLA	5	0
14	A4	814	CLA	2	0
14	A4	815	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A4	816	CLA	1	0
14	A4	817	CLA	5	0
14	A4	818	CLA	3	0
14	A4	819	CLA	3	0
14	A4	820	CLA	9	0
14	A4	821	CLA	3	0
14	A4	822	CLA	2	0
14	A4	823	CLA	1	0
14	A4	824	CLA	7	0
14	A4	825	CLA	5	0
14	A4	826	CLA	3	0
14	A4	827	CLA	11	0
14	A4	828	CLA	2	0
14	A4	829	CLA	9	0
14	A4	830	CLA	4	0
14	A4	831	CLA	5	0
14	A4	832	CLA	1	0
14	A4	833	CLA	4	0
14	A4	834	CLA	2	0
14	A4	835	CLA	4	0
14	A4	836	CLA	4	0
14	A4	837	CLA	5	0
14	A4	838	CLA	3	0
14	A4	839	CLA	1	0
14	A4	840	CLA	5	0
14	A4	841	CLA	7	0
14	A4	842	CLA	2	0
15	A4	843	PQN	2	0
16	A4	844	BCR	1	0
16	A4	845	BCR	2	0
16	A4	846	BCR	1	0
16	A4	847	BCR	3	0
16	A4	848	BCR	3	0
16	A4	849	BCR	14	0
17	A4	850	LHG	4	0
17	A4	851	LHG	3	0
18	A4	852	SF4	4	0
14	A4	853	CLA	8	0
14	A5	801	CLA	12	0
14	A5	802	CLA	5	0
14	A5	803	CLA	1	0
14	A5	804	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A5	805	CLA	13	0
14	A5	806	CLA	5	0
14	A5	807	CLA	2	0
14	A5	808	CLA	5	0
14	A5	809	CLA	3	0
14	A5	810	CLA	1	0
14	A5	811	CLA	4	0
14	A5	812	CLA	1	0
14	A5	813	CLA	2	0
14	A5	814	CLA	4	0
14	A5	815	CLA	2	0
14	A5	816	CLA	1	0
14	A5	817	CLA	1	0
14	A5	818	CLA	8	0
14	A5	819	CLA	5	0
14	A5	820	CLA	2	0
14	A5	821	CLA	6	0
14	A5	822	CLA	3	0
14	A5	823	CLA	1	0
14	A5	825	CLA	4	0
14	A5	826	CLA	5	0
14	A5	827	CLA	5	0
14	A5	828	CLA	15	0
14	A5	829	CLA	4	0
14	A5	830	CLA	10	0
14	A5	831	CLA	4	0
14	A5	832	CLA	2	0
14	A5	833	CLA	1	0
14	A5	834	CLA	4	0
14	A5	835	CLA	2	0
14	A5	836	CLA	2	0
14	A5	837	CLA	4	0
14	A5	838	CLA	5	0
14	A5	839	CLA	2	0
14	A5	840	CLA	3	0
14	A5	841	CLA	3	0
14	A5	842	CLA	5	0
14	A5	843	CLA	7	0
15	A5	844	PQN	2	0
16	A5	845	BCR	4	0
16	A5	846	BCR	2	0
16	A5	847	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A5	848	BCR	2	0
16	A5	849	BCR	3	0
16	A5	850	BCR	12	0
17	A5	851	LHG	1	0
17	A5	852	LHG	3	0
16	A5	853	BCR	1	0
18	A5	854	SF4	5	0
14	A6	1601	CLA	9	0
14	A6	1602	CLA	13	0
14	A6	1603	CLA	11	0
14	A6	1604	CLA	2	0
14	A6	1605	CLA	10	0
14	A6	1606	CLA	4	0
14	A6	1607	CLA	2	0
14	A6	1608	CLA	7	0
14	A6	1609	CLA	2	0
14	A6	1610	CLA	2	0
14	A6	1611	CLA	4	0
14	A6	1612	CLA	1	0
14	A6	1613	CLA	4	0
14	A6	1614	CLA	5	0
14	A6	1615	CLA	3	0
14	A6	1616	CLA	1	0
14	A6	1617	CLA	3	0
14	A6	1618	CLA	4	0
14	A6	1619	CLA	3	0
14	A6	1620	CLA	2	0
14	A6	1621	CLA	9	0
14	A6	1622	CLA	3	0
14	A6	1623	CLA	2	0
14	A6	1624	CLA	1	0
14	A6	1625	CLA	12	0
14	A6	1626	CLA	4	0
14	A6	1627	CLA	2	0
14	A6	1628	CLA	11	0
14	A6	1629	CLA	2	0
14	A6	1630	CLA	9	0
14	A6	1631	CLA	3	0
14	A6	1632	CLA	1	0
14	A6	1633	CLA	9	0
14	A6	1634	CLA	3	0
14	A6	1635	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A6	1636	CLA	3	0
14	A6	1637	CLA	4	0
14	A6	1638	CLA	4	0
14	A6	1639	CLA	1	0
14	A6	1640	CLA	8	0
14	A6	1641	CLA	2	0
15	A6	1642	PQN	4	0
16	A6	1643	BCR	2	0
16	A6	1644	BCR	1	0
16	A6	1645	BCR	2	0
16	A6	1646	BCR	3	0
16	A6	1647	BCR	4	0
16	A6	1648	BCR	16	0
17	A6	1649	LHG	3	0
17	A6	1650	LHG	2	0
14	A6	1651	CLA	8	0
16	A6	1652	BCR	1	0
14	B1	801	CLA	13	0
14	B1	802	CLA	16	0
14	B1	803	CLA	7	0
14	B1	804	CLA	27	0
14	B1	805	CLA	19	0
14	B1	806	CLA	11	0
14	B1	807	CLA	24	0
14	B1	808	CLA	9	0
14	B1	809	CLA	8	0
14	B1	810	CLA	3	0
14	B1	811	CLA	13	0
14	B1	814	CLA	14	0
14	B1	815	CLA	14	0
14	B1	816	CLA	3	0
14	B1	817	CLA	32	0
14	B1	818	CLA	33	0
14	B1	819	CLA	12	0
14	B1	820	CLA	13	0
14	B1	821	CLA	3	0
14	B1	822	CLA	8	0
14	B1	823	CLA	6	0
14	B1	824	CLA	7	0
14	B1	825	CLA	18	0
14	B1	826	CLA	12	0
14	B1	827	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B1	828	CLA	8	0
14	B1	829	CLA	14	0
14	B1	830	CLA	6	0
14	B1	831	CLA	5	0
14	B1	832	CLA	6	0
14	B1	833	CLA	7	0
14	B1	834	CLA	17	0
14	B1	835	CLA	3	0
14	B1	836	CLA	7	0
14	B1	837	CLA	6	0
14	B1	838	CLA	13	0
14	B1	839	CLA	5	0
14	B1	840	CLA	5	0
14	B1	841	CLA	2	0
15	B1	842	PQN	5	0
16	B1	843	BCR	1	0
16	B1	844	BCR	3	0
16	B1	845	BCR	7	0
16	B1	846	BCR	4	0
16	B1	847	BCR	6	0
16	B1	848	BCR	5	0
16	B1	849	BCR	1	0
19	B1	850	LMG	8	0
17	B1	851	LHG	2	0
16	B1	852	BCR	5	0
14	B1	853	CLA	8	0
14	B1	854	CLA	21	0
14	B2	801	CLA	13	0
14	B2	802	CLA	10	0
14	B2	803	CLA	4	0
14	B2	804	CLA	8	0
14	B2	805	CLA	7	0
14	B2	806	CLA	9	0
14	B2	807	CLA	4	0
14	B2	808	CLA	13	0
14	B2	809	CLA	10	0
14	B2	810	CLA	5	0
14	B2	812	CLA	8	0
14	B2	813	CLA	5	0
14	B2	814	CLA	4	0
14	B2	815	CLA	7	0
14	B2	816	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B2	817	CLA	3	0
14	B2	818	CLA	6	0
14	B2	819	CLA	3	0
14	B2	820	CLA	2	0
14	B2	821	CLA	7	0
14	B2	822	CLA	3	0
14	B2	823	CLA	17	0
14	B2	824	CLA	7	0
14	B2	825	CLA	7	0
14	B2	826	CLA	7	0
14	B2	827	CLA	14	0
14	B2	828	CLA	6	0
14	B2	829	CLA	5	0
14	B2	830	CLA	4	0
14	B2	831	CLA	5	0
14	B2	832	CLA	12	0
14	B2	834	CLA	2	0
14	B2	835	CLA	3	0
14	B2	836	CLA	4	0
14	B2	837	CLA	7	0
14	B2	838	CLA	7	0
14	B2	839	CLA	3	0
14	B2	840	CLA	1	0
15	B2	841	PQN	1	0
16	B2	842	BCR	4	0
16	B2	843	BCR	3	0
16	B2	844	BCR	3	0
16	B2	845	BCR	2	0
16	B2	846	BCR	4	0
16	B2	847	BCR	2	0
19	B2	848	LMG	6	0
17	B2	849	LHG	2	0
16	B2	850	BCR	2	0
14	B3	1801	CLA	11	0
14	B3	1802	CLA	14	0
14	B3	1803	CLA	14	0
14	B3	1804	CLA	12	0
14	B3	1805	CLA	9	0
14	B3	1806	CLA	5	0
14	B3	1807	CLA	12	0
14	B3	1808	CLA	7	0
14	B3	1809	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B3	1810	CLA	6	0
14	B3	1811	CLA	3	0
14	B3	1812	CLA	9	0
14	B3	1813	CLA	6	0
14	B3	1814	CLA	2	0
14	B3	1815	CLA	12	0
14	B3	1816	CLA	15	0
14	B3	1817	CLA	9	0
14	B3	1818	CLA	6	0
14	B3	1819	CLA	8	0
14	B3	1820	CLA	10	0
14	B3	1821	CLA	6	0
14	B3	1822	CLA	4	0
14	B3	1823	CLA	2	0
14	B3	1825	CLA	3	0
14	B3	1826	CLA	15	0
14	B3	1827	CLA	6	0
14	B3	1828	CLA	4	0
14	B3	1829	CLA	5	0
14	B3	1830	CLA	13	0
14	B3	1831	CLA	7	0
14	B3	1832	CLA	5	0
14	B3	1833	CLA	2	0
14	B3	1834	CLA	4	0
14	B3	1835	CLA	7	0
14	B3	1836	CLA	7	0
14	B3	1837	CLA	7	0
14	B3	1838	CLA	10	0
14	B3	1839	CLA	17	0
14	B3	1840	CLA	3	0
14	B3	1841	CLA	5	0
14	B3	1842	CLA	10	0
14	B3	1843	CLA	5	0
15	B3	1844	PQN	3	0
16	B3	1845	BCR	6	0
16	B3	1846	BCR	4	0
16	B3	1847	BCR	4	0
16	B3	1848	BCR	3	0
16	B3	1849	BCR	5	0
19	B3	1850	LMG	8	0
16	B3	1851	BCR	3	0
14	B4	801	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B4	802	CLA	12	0
14	B4	803	CLA	10	0
14	B4	804	CLA	12	0
14	B4	805	CLA	13	0
14	B4	806	CLA	3	0
14	B4	807	CLA	6	0
14	B4	808	CLA	8	0
14	B4	809	CLA	6	0
14	B4	810	CLA	8	0
14	B4	811	CLA	7	0
14	B4	812	CLA	12	0
14	B4	813	CLA	1	0
14	B4	814	CLA	1	0
14	B4	815	CLA	15	0
14	B4	816	CLA	17	0
14	B4	817	CLA	4	0
14	B4	818	CLA	8	0
14	B4	819	CLA	8	0
14	B4	820	CLA	11	0
14	B4	821	CLA	7	0
14	B4	822	CLA	2	0
14	B4	823	CLA	2	0
14	B4	825	CLA	3	0
14	B4	826	CLA	17	0
14	B4	827	CLA	3	0
14	B4	828	CLA	5	0
14	B4	829	CLA	10	0
14	B4	830	CLA	8	0
14	B4	831	CLA	7	0
14	B4	832	CLA	7	0
14	B4	833	CLA	2	0
14	B4	834	CLA	5	0
14	B4	835	CLA	7	0
14	B4	836	CLA	5	0
14	B4	837	CLA	7	0
14	B4	838	CLA	3	0
14	B4	839	CLA	7	0
14	B4	840	CLA	2	0
14	B4	841	CLA	5	0
14	B4	842	CLA	5	0
14	B4	843	CLA	2	0
15	B4	844	PQN	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B4	845	BCR	6	0
16	B4	846	BCR	6	0
16	B4	847	BCR	3	0
16	B4	848	BCR	5	0
16	B4	849	BCR	2	0
16	B4	850	BCR	1	0
19	B4	851	LMG	8	0
14	B4	852	CLA	10	0
14	B5	1801	CLA	20	0
14	B5	1802	CLA	11	0
14	B5	1803	CLA	23	0
14	B5	1804	CLA	14	0
14	B5	1805	CLA	8	0
14	B5	1806	CLA	2	0
14	B5	1807	CLA	5	0
14	B5	1808	CLA	5	0
14	B5	1809	CLA	3	0
14	B5	1810	CLA	4	0
14	B5	1811	CLA	4	0
14	B5	1812	CLA	11	0
14	B5	1815	CLA	12	0
14	B5	1816	CLA	4	0
14	B5	1817	CLA	2	0
14	B5	1818	CLA	5	0
14	B5	1819	CLA	10	0
14	B5	1820	CLA	4	0
14	B5	1821	CLA	5	0
14	B5	1822	CLA	2	0
14	B5	1823	CLA	2	0
14	B5	1824	CLA	1	0
14	B5	1825	CLA	3	0
14	B5	1826	CLA	11	0
14	B5	1827	CLA	5	0
14	B5	1828	CLA	5	0
14	B5	1829	CLA	9	0
14	B5	1830	CLA	14	0
14	B5	1831	CLA	5	0
14	B5	1832	CLA	7	0
14	B5	1833	CLA	2	0
14	B5	1834	CLA	3	0
14	B5	1835	CLA	9	0
14	B5	1836	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B5	1837	CLA	2	0
14	B5	1838	CLA	2	0
14	B5	1839	CLA	12	0
14	B5	1840	CLA	2	0
14	B5	1841	CLA	4	0
14	B5	1842	CLA	4	0
14	B5	1843	CLA	6	0
15	B5	1844	PQN	2	0
16	B5	1845	BCR	2	0
16	B5	1846	BCR	3	0
16	B5	1847	BCR	4	0
16	B5	1848	BCR	3	0
16	B5	1849	BCR	5	0
16	B5	1850	BCR	1	0
19	B5	1851	LMG	9	0
18	B6	801	SF4	7	0
14	B6	802	CLA	10	0
14	B6	803	CLA	6	0
14	B6	804	CLA	14	0
14	B6	805	CLA	4	0
14	B6	806	CLA	9	0
14	B6	807	CLA	6	0
14	B6	808	CLA	4	0
14	B6	809	CLA	8	0
14	B6	810	CLA	11	0
14	B6	811	CLA	3	0
14	B6	813	CLA	8	0
14	B6	814	CLA	3	0
14	B6	815	CLA	2	0
14	B6	816	CLA	3	0
14	B6	817	CLA	9	0
14	B6	818	CLA	7	0
14	B6	819	CLA	8	0
14	B6	820	CLA	2	0
14	B6	821	CLA	4	0
14	B6	822	CLA	6	0
14	B6	823	CLA	3	0
14	B6	824	CLA	16	0
14	B6	825	CLA	8	0
14	B6	826	CLA	6	0
14	B6	827	CLA	5	0
14	B6	828	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B6	829	CLA	6	0
14	B6	830	CLA	6	0
14	B6	831	CLA	2	0
14	B6	832	CLA	7	0
14	B6	833	CLA	7	0
14	B6	835	CLA	3	0
14	B6	836	CLA	3	0
14	B6	837	CLA	11	0
14	B6	838	CLA	4	0
14	B6	839	CLA	5	0
14	B6	840	CLA	3	0
14	B6	841	CLA	2	0
15	B6	842	PQN	1	0
16	B6	843	BCR	1	0
16	B6	844	BCR	3	0
16	B6	845	BCR	4	0
16	B6	846	BCR	1	0
16	B6	847	BCR	4	0
19	B6	848	LMG	10	0
17	B6	849	LHG	2	0
16	B6	850	BCR	4	0
18	C1	101	SF4	5	0
18	C1	102	SF4	7	0
18	C2	101	SF4	7	0
18	C2	102	SF4	6	0
18	C3	101	SF4	8	0
18	C3	102	SF4	4	0
18	C4	101	SF4	4	0
18	C4	102	SF4	3	0
18	C5	101	SF4	7	0
18	C5	102	SF4	6	0
18	C6	101	SF4	4	0
18	C6	102	SF4	4	0
14	F1	1301	CLA	1	0
16	F1	1302	BCR	2	0
16	F2	201	BCR	3	0
14	F2	202	CLA	4	0
16	F2	203	BCR	2	0
14	F2	204	CLA	9	0
16	F3	201	BCR	2	0
14	F3	202	CLA	3	0
16	F3	203	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	F4	201	BCR	9	0
14	F4	202	CLA	7	0
16	F4	203	BCR	1	0
16	F4	204	BCR	5	0
14	F5	1301	CLA	4	0
16	F5	1302	BCR	2	0
16	F6	201	BCR	2	0
14	F6	202	CLA	14	0
16	F6	203	BCR	1	0
14	I1	101	CLA	3	0
16	I1	102	BCR	3	0
16	I1	103	BCR	9	0
16	I2	101	BCR	5	0
16	I3	101	BCR	3	0
16	I3	102	BCR	4	0
16	I4	101	BCR	1	0
16	I4	102	BCR	11	0
16	I5	101	BCR	3	0
16	I5	102	BCR	2	0
14	I6	101	CLA	2	0
16	I6	102	BCR	3	0
14	J1	101	CLA	7	0
14	J1	102	CLA	5	0
16	J1	103	BCR	3	0
16	J1	104	BCR	10	0
14	J2	101	CLA	6	0
16	J2	102	BCR	4	0
16	J2	103	BCR	6	0
14	J3	101	CLA	6	0
16	J3	103	BCR	4	0
16	J3	104	BCR	2	0
14	J4	101	CLA	8	0
14	J4	102	CLA	4	0
16	J4	103	BCR	4	0
16	J4	104	BCR	9	0
14	J5	101	CLA	6	0
14	J5	102	CLA	3	0
16	J5	103	BCR	5	0
16	J5	104	BCR	13	0
16	J5	105	BCR	4	0
14	J6	1101	CLA	4	0
14	J6	1102	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	J6	1104	BCR	6	0
16	J6	1105	BCR	8	0
14	K1	1401	CLA	4	0
14	K2	1401	CLA	3	0
14	K3	1401	CLA	1	0
14	K4	1401	CLA	3	0
14	K5	101	CLA	1	0
14	K6	1401	CLA	2	0
14	L1	201	CLA	4	0
14	L1	202	CLA	4	0
16	L1	203	BCR	3	0
14	L1	205	CLA	8	0
14	L1	206	CLA	5	0
14	L1	207	CLA	6	0
16	L1	209	BCR	9	0
16	L2	201	BCR	5	0
14	L2	202	CLA	6	0
16	L2	203	BCR	2	0
14	L2	205	CLA	3	0
14	L2	206	CLA	7	0
14	L2	207	CLA	8	0
16	L2	208	BCR	3	0
16	L3	201	BCR	4	0
14	L3	202	CLA	4	0
14	L3	203	CLA	13	0
14	L3	204	CLA	7	0
14	L3	205	CLA	9	0
16	L3	206	BCR	5	0
14	L4	201	CLA	11	0
14	L4	203	CLA	11	0
14	L4	204	CLA	8	0
14	L4	205	CLA	9	0
16	L4	206	BCR	5	0
16	L4	208	BCR	8	0
16	L5	201	BCR	6	0
14	L5	202	CLA	5	0
14	L5	203	CLA	11	0
14	L5	204	CLA	11	0
14	L5	205	CLA	8	0
14	L5	206	CLA	7	0
16	L5	207	BCR	5	0
16	L6	201	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	L6	202	CLA	6	0
14	L6	203	CLA	11	0
16	L6	204	BCR	1	0
14	L6	206	CLA	11	0
14	L6	207	CLA	8	0
14	L6	208	CLA	15	0
16	L6	209	BCR	4	0
14	M1	1201	CLA	3	0
16	M1	1202	BCR	2	0
14	M2	1201	CLA	1	0
16	M2	1202	BCR	2	0
14	M3	1601	CLA	11	0
16	M3	1602	BCR	9	0
16	M4	101	BCR	6	0
16	M5	101	BCR	3	0
14	M6	1201	CLA	2	0
16	M6	1202	BCR	2	0
14	X1	1701	CLA	2	0
14	X2	1701	CLA	6	0
17	X3	101	LHG	6	0
14	X3	102	CLA	1	0
17	X4	101	LHG	1	0
14	X4	102	CLA	16	0
14	X5	101	CLA	2	0
14	X6	1701	CLA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A1	740/755 (98%)	0.68	92 (12%) 4 4	150, 166, 177, 185	0
1	A2	740/755 (98%)	0.20	41 (5%) 25 19	150, 161, 172, 180	0
1	A3	740/755 (98%)	0.19	30 (4%) 37 28	150, 157, 168, 179	0
1	A4	740/755 (98%)	0.27	61 (8%) 11 9	150, 166, 178, 187	0
1	A5	740/755 (98%)	0.18	34 (4%) 32 24	150, 160, 171, 179	0
1	A6	740/755 (98%)	0.22	28 (3%) 40 30	150, 159, 169, 180	0
2	B1	739/740 (99%)	0.40	58 (7%) 13 9	150, 165, 176, 187	0
2	B2	739/740 (99%)	-0.01	12 (1%) 72 61	150, 159, 171, 179	0
2	B3	739/740 (99%)	0.09	17 (2%) 60 49	150, 160, 171, 184	0
2	B4	739/740 (99%)	0.10	19 (2%) 56 44	150, 163, 174, 182	0
2	B5	739/740 (99%)	0.26	36 (4%) 29 22	150, 161, 173, 181	0
2	B6	739/740 (99%)	0.10	20 (2%) 54 43	150, 161, 172, 180	0
3	C1	80/80 (100%)	1.12	22 (27%) 0 0	153, 166, 178, 182	0
3	C2	80/80 (100%)	0.15	1 (1%) 77 67	150, 159, 167, 172	0
3	C3	80/80 (100%)	0.36	5 (6%) 20 14	150, 159, 169, 175	0
3	C4	80/80 (100%)	0.49	7 (8%) 10 7	150, 163, 172, 180	0
3	C5	80/80 (100%)	0.75	13 (16%) 1 2	150, 161, 170, 173	0
3	C6	80/80 (100%)	0.38	6 (7%) 14 10	150, 160, 171, 178	0
4	D1	138/138 (100%)	0.28	10 (7%) 15 11	151, 163, 172, 179	0
4	D2	138/138 (100%)	-0.11	2 (1%) 75 65	151, 161, 171, 180	0
4	D3	138/138 (100%)	-0.17	1 (0%) 87 81	150, 160, 170, 173	0
4	D4	138/138 (100%)	-0.15	3 (2%) 62 51	151, 165, 174, 185	0
4	D5	138/138 (100%)	0.28	12 (8%) 10 7	151, 162, 171, 178	0
4	D6	138/138 (100%)	0.19	6 (4%) 35 26	152, 162, 174, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	E1	69/75 (92%)	1.23	19 (27%) 0 0	160, 170, 179, 184	0
5	E2	69/75 (92%)	0.43	7 (10%) 7 5	154, 164, 173, 178	0
5	E3	69/75 (92%)	0.16	4 (5%) 23 17	150, 162, 170, 175	0
5	E4	69/75 (92%)	0.68	14 (20%) 1 1	157, 170, 179, 182	0
5	E5	69/75 (92%)	0.62	8 (11%) 4 4	154, 167, 177, 179	0
5	E6	69/75 (92%)	0.86	10 (14%) 2 2	151, 165, 173, 178	0
6	F1	141/164 (85%)	1.01	26 (18%) 1 1	157, 171, 179, 184	0
6	F2	141/164 (85%)	0.12	4 (2%) 53 41	155, 168, 177, 181	0
6	F3	141/164 (85%)	0.39	10 (7%) 16 11	152, 165, 176, 179	0
6	F4	141/164 (85%)	0.59	18 (12%) 3 3	154, 170, 179, 187	0
6	F5	141/164 (85%)	0.18	8 (5%) 24 18	152, 166, 175, 185	0
6	F6	141/164 (85%)	0.32	13 (9%) 9 7	153, 166, 174, 182	0
7	I1	38/38 (100%)	0.02	0 100 100	150, 157, 166, 169	0
7	I2	38/38 (100%)	0.19	1 (2%) 56 44	150, 155, 166, 168	0
7	I3	38/38 (100%)	-0.07	0 100 100	150, 153, 163, 167	0
7	I4	38/38 (100%)	0.17	0 100 100	150, 156, 164, 169	0
7	I5	38/38 (100%)	0.10	0 100 100	150, 156, 165, 170	0
7	I6	38/38 (100%)	0.04	0 100 100	150, 154, 172, 172	0
8	J1	41/41 (100%)	0.26	5 (12%) 4 4	158, 170, 179, 184	0
8	J2	41/41 (100%)	0.27	2 (4%) 29 22	156, 166, 175, 185	0
8	J3	41/41 (100%)	0.18	2 (4%) 29 22	156, 165, 173, 178	0
8	J4	41/41 (100%)	0.77	5 (12%) 4 4	159, 170, 177, 185	0
8	J5	41/41 (100%)	0.24	1 (2%) 59 47	153, 166, 177, 179	0
8	J6	41/41 (100%)	-0.26	0 100 100	155, 164, 175, 179	0
9	K1	46/83 (55%)	-0.02	3 (6%) 19 13	151, 172, 184, 190	0
9	K2	46/83 (55%)	-0.55	0 100 100	155, 166, 173, 183	0
9	K3	46/83 (55%)	-0.14	3 (6%) 19 13	150, 163, 173, 180	0
9	K4	46/83 (55%)	-0.22	0 100 100	158, 175, 182, 184	0
9	K5	46/83 (55%)	-0.08	4 (8%) 10 7	156, 167, 178, 184	0
9	K6	46/83 (55%)	-0.32	3 (6%) 19 13	151, 162, 173, 179	0
10	L1	151/154 (98%)	0.23	5 (3%) 46 35	150, 154, 169, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
10	L2	151/154 (98%)	0.30	5 (3%) 46 35	150, 155, 167, 174	0
10	L3	151/154 (98%)	0.16	2 (1%) 77 67	150, 155, 166, 171	0
10	L4	151/154 (98%)	0.28	2 (1%) 77 67	150, 156, 172, 185	0
10	L5	151/154 (98%)	0.15	1 (0%) 87 81	150, 156, 166, 177	0
10	L6	151/154 (98%)	0.26	2 (1%) 77 67	150, 154, 170, 178	0
11	M1	31/31 (100%)	-0.08	0 100 100	150, 160, 173, 177	0
11	M2	31/31 (100%)	-0.05	1 (3%) 47 35	151, 157, 167, 173	0
11	M3	31/31 (100%)	-0.13	1 (3%) 47 35	151, 160, 169, 172	0
11	M4	31/31 (100%)	0.14	1 (3%) 47 35	150, 160, 166, 171	0
11	M5	31/31 (100%)	-0.14	0 100 100	150, 158, 166, 170	0
11	M6	31/31 (100%)	-0.12	0 100 100	150, 160, 169, 171	0
12	X1	29/35 (82%)	0.81	3 (10%) 6 5	165, 172, 183, 185	0
12	X2	29/35 (82%)	-0.48	1 (3%) 45 34	156, 166, 173, 176	0
12	X3	29/35 (82%)	0.24	3 (10%) 6 5	154, 165, 176, 186	0
12	X4	29/35 (82%)	0.01	2 (6%) 17 11	159, 169, 181, 187	0
12	X5	29/35 (82%)	-0.08	0 100 100	153, 166, 179, 185	0
12	X6	29/35 (82%)	-0.16	2 (6%) 17 11	158, 166, 174, 178	0
13	P1	97/97 (100%)	1.02	18 (18%) 1 1	156, 171, 180, 185	2 (2%)
13	P2	97/97 (100%)	0.53	14 (14%) 2 2	153, 169, 179, 185	2 (2%)
13	P3	97/97 (100%)	0.37	6 (6%) 20 15	151, 163, 172, 177	2 (2%)
13	P4	97/97 (100%)	0.13	5 (5%) 27 21	156, 171, 180, 186	2 (2%)
13	P5	97/97 (100%)	0.65	13 (13%) 3 3	153, 170, 181, 187	2 (2%)
13	P6	97/97 (100%)	0.09	2 (2%) 63 52	153, 164, 175, 179	2 (2%)
All	All	14040/14586 (96%)	0.24	795 (5%) 24 18	150, 162, 175, 190	12 (0%)

All (795) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B4	571	GLY	9.5
1	A1	40	ARG	8.0
2	B4	572	GLY	7.9
6	F1	50	HIS	7.6
2	B4	570	ARG	6.9
6	F4	3	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	A1	36	ARG	6.7
6	F1	25	THR	6.7
1	A6	43	GLN	6.7
4	D1	1	THR	6.6
13	P1	60	SER	6.6
1	A4	43	GLN	6.4
5	E4	52	ALA	6.4
2	B1	512	ASN	6.3
5	E1	46	THR	6.3
6	F6	1	ASP	6.3
1	A1	37	THR	6.3
2	B1	307	LYS	6.2
1	A1	692	SER	6.0
1	A1	379	PRO	5.9
1	A4	574	PHE	5.9
6	F4	1	ASP	5.8
1	A2	50	ASN	5.7
6	F1	24	THR	5.7
5	E4	45	TYR	5.7
5	E4	53	SER	5.6
2	B5	572	GLY	5.6
1	A4	719	PRO	5.5
2	B4	573	THR	5.5
2	B1	259	GLY	5.5
1	A4	585	GLY	5.5
1	A1	573	GLY	5.4
5	E1	45	TYR	5.4
6	F1	49	PRO	5.3
5	E5	31	GLY	5.3
1	A4	720	ARG	5.3
1	A1	191	GLN	5.2
1	A1	13	ARG	5.1
13	P1	1	ALA	5.1
2	B1	570	ARG	5.1
1	A4	575	ARG	5.1
13	P5	36	LEU	5.0
5	E4	47	GLY	5.0
2	B1	453	GLU	5.0
1	A4	718	GLN	4.9
11	M4	31	LYS	4.9
1	A1	571	ASN	4.9
1	A4	693	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
12	X3	7	PRO	4.9
5	E4	54	GLY	4.9
1	A1	39	ALA	4.8
5	E1	53	SER	4.8
5	E1	52	ALA	4.8
6	F1	26	ALA	4.8
1	A1	561	ARG	4.7
1	A6	40	ARG	4.7
2	B4	569	GLY	4.7
1	A1	417	VAL	4.6
4	D5	26	LYS	4.6
13	P2	67	ASP	4.6
5	E4	46	THR	4.6
6	F1	44	GLY	4.6
1	A4	571	ASN	4.6
1	A4	579	ASP	4.6
1	A4	159	TYR	4.6
5	E4	51	SER	4.5
6	F3	3	ALA	4.5
6	F5	58	SER	4.5
1	A4	573	GLY	4.5
6	F2	1	ASP	4.5
3	C1	49	GLY	4.5
2	B5	477	PHE	4.5
1	A1	721	ALA	4.5
5	E1	55	VAL	4.4
2	B1	85	PRO	4.4
6	F6	2	VAL	4.4
13	P5	22	ASP	4.4
1	A4	694	ARG	4.3
13	P2	32	GLN	4.3
13	P1	61	ASP	4.3
1	A5	719	PRO	4.3
1	A1	416	MET	4.3
2	B1	408	GLY	4.3
1	A4	576	PHE	4.2
1	A3	40	ARG	4.2
6	F1	46	ASP	4.2
6	F1	45	GLU	4.2
6	F4	2	VAL	4.2
3	C5	80	TYR	4.2
1	A1	728	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
2	B1	520	PRO	4.2
1	A4	40	ARG	4.2
2	B1	485	ASP	4.2
12	X3	8	THR	4.1
1	A4	590	SER	4.1
6	F4	27	ASP	4.1
1	A4	572	LEU	4.1
1	A1	316	ARG	4.1
13	P5	95	GLU	4.1
6	F1	95	ASN	4.1
6	F1	37	ARG	4.1
5	E2	52	ALA	4.1
5	E4	48	TYR	4.0
2	B1	406	ASN	4.0
2	B6	479	THR	4.0
5	E1	31	GLY	4.0
1	A1	283	GLY	4.0
1	A1	346	GLU	4.0
1	A1	317	THR	4.0
2	B1	484	PRO	4.0
5	E1	54	GLY	4.0
1	A1	426	GLN	4.0
6	F1	2	VAL	4.0
13	P1	58	ASP	4.0
12	X6	35	ALA	4.0
8	J4	25	ILE	3.9
2	B1	572	GLY	3.9
2	B2	548	ARG	3.9
5	E6	30	PRO	3.9
2	B2	406	ASN	3.9
3	C1	12	GLY	3.9
5	E3	54	GLY	3.9
1	A4	59	ASP	3.9
6	F4	95	ASN	3.9
9	K5	41	PRO	3.9
6	F5	1	ASP	3.8
1	A4	228	ASP	3.8
1	A4	592	TRP	3.8
2	B1	569	GLY	3.8
5	E2	53	SER	3.8
2	B5	510	GLY	3.8
6	F6	141	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
5	E6	29	THR	3.8
2	B5	475	TYR	3.8
6	F6	3	ALA	3.7
4	D3	1	THR	3.7
3	C1	68	LEU	3.7
5	E2	32	VAL	3.7
10	L2	72	ASP	3.7
6	F4	4	GLY	3.7
2	B5	609	GLU	3.7
5	E5	52	ALA	3.7
13	P1	7	LEU	3.7
1	A1	698	GLN	3.7
1	A1	694	ARG	3.7
6	F6	5	LEU	3.7
2	B4	218	PRO	3.7
2	B4	566	ASP	3.6
1	A1	348	LEU	3.6
9	K5	42	GLY	3.6
5	E4	50	GLY	3.6
1	A1	735	TYR	3.6
3	C1	64	ILE	3.6
1	A6	278	PHE	3.6
5	E6	1	VAL	3.6
2	B6	405	GLN	3.6
6	F1	51	LEU	3.6
3	C5	62	LEU	3.6
1	A2	36	ARG	3.6
13	P4	63	SER	3.6
1	A2	237	PRO	3.5
8	J1	40	PRO	3.5
1	A6	692	SER	3.5
1	A4	31	PRO	3.5
1	A2	31	PRO	3.5
1	A3	37	THR	3.5
3	C6	2	HIS	3.5
5	E4	43	VAL	3.5
1	A4	569	LYS	3.4
5	E6	45	TYR	3.4
1	A6	37	THR	3.4
3	C5	32	GLY	3.4
6	F5	2	VAL	3.4
9	K6	39	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	B5	291	ARG	3.4
6	F1	47	GLY	3.4
1	A1	347	VAL	3.4
1	A4	696	TYR	3.4
4	D1	42	PRO	3.4
13	P1	59	GLN	3.4
1	A3	316	ARG	3.4
1	A4	591	GLY	3.4
1	A1	572	LEU	3.4
2	B6	477	PHE	3.4
1	A4	583	ARG	3.3
1	A1	14	VAL	3.3
1	A1	279	LEU	3.3
1	A2	49	TRP	3.3
12	X1	33	ALA	3.3
13	P2	36	LEU	3.3
1	A4	581	PRO	3.3
1	A1	261	PHE	3.3
4	D5	25	GLU	3.3
1	A3	244	LEU	3.3
1	A6	41	GLY	3.3
5	E2	33	LYS	3.3
1	A2	114	ALA	3.3
2	B3	477	PHE	3.3
2	B1	479	THR	3.3
1	A4	728	ARG	3.3
1	A1	63	SER	3.3
1	A4	44	THR	3.3
12	X6	7	PRO	3.3
5	E5	33	LYS	3.3
2	B3	313	LYS	3.3
1	A1	591	GLY	3.2
1	A1	38	LEU	3.2
1	A1	598	GLY	3.2
1	A4	671	ALA	3.2
2	B1	306	ALA	3.2
1	A1	568	ASP	3.2
2	B1	318	PHE	3.2
4	D1	2	THR	3.2
1	A4	692	SER	3.2
2	B6	247	GLN	3.2
1	A1	350	THR	3.2

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Mol	Chain	Res	Type	RSRZ
5	E4	49	SER	3.2
6	F1	9	LYS	3.2
6	F1	38	TYR	3.2
1	A2	37	THR	3.2
1	A5	191	GLN	3.2
2	B2	418	LYS	3.2
1	A4	586	THR	3.2
1	A1	74	SER	3.2
1	A3	96	LYS	3.2
1	A5	561	ARG	3.2
3	C1	39	ALA	3.2
2	B2	407	LYS	3.2
6	F1	141	ARG	3.1
8	J3	41	LEU	3.1
2	B1	521	GLY	3.1
3	C5	78	LEU	3.1
1	A1	318	ASN	3.1
1	A2	40	ARG	3.1
1	A2	692	SER	3.1
1	A2	727	GLY	3.1
3	C5	7	TYR	3.1
8	J1	35	ASP	3.1
1	A1	722	LEU	3.1
2	B1	454	LYS	3.1
8	J1	41	LEU	3.1
2	B1	228	ASN	3.1
3	C6	71	GLU	3.1
1	A1	187	LEU	3.1
2	B1	258	GLY	3.1
4	D5	12	GLY	3.1
13	P6	32	GLN	3.1
1	A4	504	ASN	3.1
13	P5	88	ILE	3.1
5	E3	53	SER	3.1
4	D1	40	GLU	3.1
1	A3	284	GLY	3.1
6	F3	137	THR	3.1
1	A6	379	PRO	3.1
1	A6	499	GLY	3.1
3	C1	60	ASP	3.1
2	B5	418	LYS	3.1
9	K1	39	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	B3	233	ALA	3.1
2	B3	258	GLY	3.1
1	A3	720	ARG	3.1
1	A1	41	GLY	3.0
5	E1	44	ASN	3.0
2	B1	551	LYS	3.0
13	P2	38	PHE	3.0
1	A2	142	GLY	3.0
13	P2	66	ASP	3.0
2	B3	472	LYS	3.0
5	E1	3	ARG	3.0
5	E1	23	VAL	3.0
1	A5	693	GLY	3.0
2	B6	548	ARG	3.0
2	B3	307	LYS	3.0
8	J1	33	TYR	3.0
2	B1	313	LYS	3.0
6	F6	96	GLU	3.0
1	A2	352	TRP	3.0
4	D5	108	GLY	3.0
2	B1	314	VAL	3.0
6	F1	34	ARG	3.0
1	A6	588	GLN	3.0
3	C1	48	VAL	3.0
2	B1	252	ALA	3.0
6	F1	3	ALA	3.0
1	A1	193	VAL	3.0
1	A3	379	PRO	3.0
1	A2	278	PHE	3.0
1	A3	317	THR	3.0
1	A4	716	ALA	3.0
5	E3	55	VAL	3.0
1	A2	54	LEU	3.0
2	B5	306	ALA	3.0
1	A2	392	SER	2.9
6	F1	40	GLN	2.9
6	F1	27	ASP	2.9
1	A1	560	ALA	2.9
3	C5	79	ALA	2.9
13	P1	15	THR	2.9
1	A4	229	ALA	2.9
1	A5	14	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A3	588	GLN	2.9
1	A1	683	TRP	2.9
4	D5	13	SER	2.9
2	B3	475	TYR	2.9
1	A4	721	ALA	2.9
1	A1	562	SER	2.9
3	C1	61	PHE	2.9
2	B3	239	ALA	2.9
1	A1	737	LEU	2.9
2	B1	483	ASN	2.9
2	B3	257	LEU	2.9
6	F4	5	LEU	2.9
6	F3	141	ARG	2.9
2	B1	477	PHE	2.9
6	F3	134	ASN	2.9
2	B3	300	ILE	2.9
3	C1	38	ILE	2.9
6	F6	140	PRO	2.9
3	C1	2	HIS	2.9
5	E6	27	ASP	2.9
2	B6	333	LEU	2.9
2	B5	570	ARG	2.9
1	A3	243	ILE	2.9
12	X1	32	ALA	2.9
2	B5	509	SER	2.9
6	F5	3	ALA	2.9
2	B3	708	ILE	2.9
2	B5	511	THR	2.9
13	P5	14	GLU	2.9
6	F3	136	ILE	2.9
1	A4	675	LEU	2.8
10	L5	64	LYS	2.8
1	A1	17	ASP	2.8
1	A4	697	TRP	2.8
2	B4	475	TYR	2.8
1	A1	693	GLY	2.8
1	A4	353	HIS	2.8
13	P5	12	GLY	2.8
3	C1	5	LYS	2.8
6	F4	49	PRO	2.8
2	B3	252	ALA	2.8
1	A1	278	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B3	399	ARG	2.8
1	A5	13	ARG	2.8
2	B5	292	THR	2.8
5	E6	52	ALA	2.8
13	P4	97	TYR	2.8
1	A1	132	GLY	2.8
1	A5	59	ASP	2.8
6	F3	133	ASP	2.8
1	A5	183	ARG	2.8
1	A1	251	GLU	2.8
1	A2	379	PRO	2.8
2	B1	267	LEU	2.8
2	B1	407	LYS	2.8
2	B2	237	ASP	2.8
1	A4	32	GLY	2.8
2	B5	479	THR	2.8
1	A3	283	GLY	2.8
3	C1	62	LEU	2.8
6	F2	25	THR	2.8
6	F4	22	VAL	2.8
2	B5	300	ILE	2.8
4	D5	119	ILE	2.8
1	A4	191	GLN	2.8
8	J5	41	LEU	2.8
5	E6	31	GLY	2.8
6	F1	48	LEU	2.8
1	A5	321	ILE	2.8
2	B1	272	MET	2.8
1	A1	30	LYS	2.8
2	B1	584	LEU	2.8
1	A1	596	PHE	2.8
2	B5	240	SER	2.8
5	E6	53	SER	2.8
8	J4	26	LEU	2.8
2	B5	234	GLN	2.8
2	B1	471	GLY	2.8
2	B5	599	TYR	2.8
5	E5	32	VAL	2.8
1	A6	42	PRO	2.8
4	D6	46	ALA	2.7
12	X4	10	ALA	2.7
1	A1	574	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
6	F1	102	ASP	2.7
1	A5	720	ARG	2.7
1	A1	119	PRO	2.7
2	B2	218	PRO	2.7
1	A5	416	MET	2.7
2	B5	598	PHE	2.7
1	A6	151	GLY	2.7
2	B6	408	GLY	2.7
10	L1	15	GLY	2.7
10	L1	13	PHE	2.7
6	F4	23	ASN	2.7
2	B1	739	PHE	2.7
2	B1	234	GLN	2.7
5	E1	1	VAL	2.7
6	F2	141	ARG	2.7
1	A5	515	GLY	2.7
2	B1	452	PRO	2.7
1	A3	261	PHE	2.7
1	A6	31	PRO	2.7
3	C1	70	ALA	2.7
6	F4	47	GLY	2.7
9	K3	57	PRO	2.7
6	F6	137	THR	2.7
2	B1	372	ALA	2.7
2	B1	253	ILE	2.7
2	B4	234	GLN	2.7
5	E1	15	TYR	2.7
1	A6	583	ARG	2.7
4	D5	61	LYS	2.7
1	A4	698	GLN	2.7
5	E1	26	VAL	2.7
6	F5	49	PRO	2.7
1	A1	188	GLU	2.7
2	B1	513	SER	2.7
2	B6	330	ASN	2.7
13	P1	26	LEU	2.7
1	A4	37	THR	2.7
2	B1	522	ASP	2.6
2	B2	109	SER	2.7
9	K5	37	ARG	2.7
13	P5	23	GLU	2.7
6	F1	133	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	C5	38	ILE	2.6
2	B1	511	THR	2.6
1	A2	59	ASP	2.6
5	E1	47	GLY	2.6
1	A4	560	ALA	2.6
1	A2	505	ALA	2.6
4	D6	12	GLY	2.6
1	A5	288	VAL	2.6
10	L4	72	ASP	2.6
3	C5	67	TYR	2.6
1	A4	561	ARG	2.6
13	P2	35	ASP	2.6
4	D2	110	GLU	2.6
1	A1	392	SER	2.6
1	A6	155	GLU	2.6
9	K6	40	GLY	2.6
1	A5	721	ALA	2.6
10	L3	140	GLU	2.6
13	P2	30	GLU	2.6
13	P2	71	GLU	2.6
6	F1	94	ALA	2.6
1	A2	74	SER	2.6
2	B1	315	GLU	2.6
1	A2	51	LEU	2.6
2	B4	575	ASP	2.6
1	A2	389	THR	2.6
2	B4	568	PRO	2.6
1	A1	43	GLN	2.6
3	C5	31	ASP	2.6
1	A1	73	PHE	2.6
5	E1	51	SER	2.6
6	F4	28	PRO	2.6
3	C1	1	ALA	2.6
1	A4	724	ILE	2.6
1	A4	589	VAL	2.6
6	F6	138	VAL	2.6
4	D6	1	THR	2.6
13	P3	83	ARG	2.6
1	A5	716	ALA	2.6
2	B6	359	PRO	2.6
1	A5	709	ASN	2.6
3	C4	64	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A1	272	TRP	2.6
1	A1	352	TRP	2.6
2	B5	508	ASN	2.6
1	A1	743	THR	2.6
1	A3	722	LEU	2.6
1	A5	583	ARG	2.5
1	A1	734	HIS	2.5
2	B2	401	TYR	2.5
5	E5	51	SER	2.5
1	A6	516	ASP	2.5
2	B1	552	LEU	2.5
4	D6	45	GLY	2.5
9	K1	38	GLY	2.5
2	B6	406	ASN	2.5
2	B6	475	TYR	2.5
9	K3	56	LEU	2.5
1	A4	584	GLY	2.5
1	A2	141	SER	2.5
1	A1	720	ARG	2.5
2	B1	226	THR	2.5
1	A1	35	ASP	2.5
2	B1	607	VAL	2.5
11	M3	31	LYS	2.5
4	D5	64	CYS	2.5
13	P3	13	SER	2.5
5	E1	2	GLN	2.5
3	C1	80	TYR	2.5
1	A4	352	TRP	2.5
2	B1	331	ASN	2.5
2	B3	171	GLU	2.5
8	J2	41	LEU	2.5
1	A3	183	ARG	2.5
1	A6	152	ILE	2.5
1	A1	18	ASN	2.5
2	B5	390	PHE	2.5
2	B4	511	THR	2.5
2	B1	231	VAL	2.5
6	F3	128	GLU	2.5
6	F6	95	ASN	2.5
2	B3	296	ILE	2.5
2	B1	508	ASN	2.5
6	F4	34	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	B5	573	THR	2.5
9	K5	57	PRO	2.4
10	L3	154	ASN	2.4
1	A2	586	THR	2.4
1	A5	152	ILE	2.4
13	P5	35	ASP	2.4
1	A5	418	ARG	2.4
2	B5	603	LYS	2.4
13	P5	13	SER	2.4
13	P5	1	ALA	2.4
1	A1	690	LEU	2.4
1	A6	150	SER	2.4
1	A1	732	VAL	2.4
1	A2	579	ASP	2.4
2	B1	503	TRP	2.4
10	L1	12	PRO	2.4
13	P2	92	GLN	2.4
2	B1	292	THR	2.4
7	I2	4	SER	2.4
1	A4	60	THR	2.4
2	B1	497	ASN	2.4
8	J4	24	GLY	2.4
9	K1	40	GLY	2.4
13	P1	20	PRO	2.4
2	B4	576	ILE	2.4
2	B2	545	LEU	2.4
6	F3	53	VAL	2.4
1	A1	156	PHE	2.4
1	A1	186	LYS	2.4
1	A1	189	TRP	2.4
3	C3	2	HIS	2.4
13	P2	70	ILE	2.4
1	A4	722	LEU	2.4
1	A1	274	ALA	2.4
3	C1	69	GLY	2.4
13	P4	61	ASP	2.4
3	C1	11	ILE	2.4
3	C5	30	TRP	2.4
6	F5	40	GLN	2.4
12	X2	7	PRO	2.4
1	A4	702	GLU	2.4
1	A5	437	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B4	739	PHE	2.4
6	F5	136	ILE	2.4
1	A4	520	VAL	2.4
3	C3	4	VAL	2.4
1	A6	23	THR	2.4
2	B4	291	ARG	2.4
1	A3	279	LEU	2.4
2	B5	672	SER	2.4
1	A3	676	PHE	2.4
3	C5	64	ILE	2.4
1	A3	318	ASN	2.4
3	C4	38	ILE	2.4
3	C3	41	SER	2.4
1	A3	352	TRP	2.4
3	C1	65	ARG	2.4
4	D5	44	ALA	2.4
6	F1	136	ILE	2.4
1	A2	228	ASP	2.4
3	C5	39	ALA	2.4
5	E3	45	TYR	2.4
13	P1	79	VAL	2.4
1	A1	733	ALA	2.4
1	A3	152	ILE	2.4
1	A4	243	ILE	2.3
5	E2	31	GLY	2.3
6	F3	2	VAL	2.3
5	E2	54	GLY	2.3
2	B2	547	ALA	2.3
1	A3	285	LEU	2.3
13	P5	9	ARG	2.3
2	B5	682	GLU	2.3
1	A5	696	TYR	2.3
1	A1	581	PRO	2.3
1	A4	588	GLN	2.3
3	C4	70	ALA	2.3
6	F5	57	LEU	2.3
3	C4	2	HIS	2.3
1	A1	194	GLU	2.3
1	A3	661	VAL	2.3
1	A6	121	VAL	2.3
2	B1	482	SER	2.3
13	P1	25	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A1	389	THR	2.3
3	C1	67	TYR	2.3
6	F4	111	LEU	2.3
1	A6	498	PRO	2.3
1	A1	736	LEU	2.3
2	B6	407	LYS	2.3
3	C4	61	PHE	2.3
4	D1	26	LYS	2.3
6	F6	93	GLU	2.3
13	P2	93	GLU	2.3
2	B4	299	SER	2.3
3	C4	62	LEU	2.3
13	P5	96	LEU	2.3
4	D1	53	GLU	2.3
13	P4	38	PHE	2.3
10	L6	72	ASP	2.3
1	A1	65	LEU	2.3
1	A6	279	LEU	2.3
1	A3	693	GLY	2.3
5	E1	48	TYR	2.3
5	E5	30	PRO	2.3
4	D4	1	THR	2.3
1	A1	374	MET	2.3
13	P1	80	ALA	2.3
13	P1	46	SER	2.3
1	A1	66	GLU	2.3
3	C3	5	LYS	2.3
3	C6	38	ILE	2.3
13	P1	54	GLU	2.3
13	P2	63	SER	2.3
2	B2	485	ASP	2.3
6	F4	43	CYS	2.3
1	A1	420	TYR	2.3
1	A2	382	TYR	2.3
1	A6	515	GLY	2.3
1	A5	413	ALA	2.3
2	B6	570	ARG	2.3
2	B5	262	PRO	2.3
5	E1	24	ALA	2.3
6	F4	42	LEU	2.3
1	A1	502	ALA	2.3
2	B5	233	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
9	K6	41	PRO	2.3
1	A2	295	SER	2.2
1	A6	114	ALA	2.2
1	A3	696	TYR	2.2
1	A5	724	ILE	2.2
4	D4	45	GLY	2.2
2	B1	218	PRO	2.2
2	B5	239	ALA	2.2
12	X3	31	PHE	2.2
1	A1	579	ASP	2.2
5	E1	25	SER	2.2
2	B1	256	PHE	2.2
1	A5	525	ALA	2.2
3	C3	64	ILE	2.2
3	C5	61	PHE	2.2
1	A4	226	LEU	2.2
2	B5	171	GLU	2.2
2	B3	395	ILE	2.2
2	B4	453	GLU	2.2
2	B6	226	THR	2.2
1	A6	65	LEU	2.2
1	A5	153	THR	2.2
2	B1	499	TRP	2.2
6	F2	10	ASP	2.2
1	A2	726	GLN	2.2
2	B5	620	THR	2.2
10	L6	141	ASN	2.2
13	P1	62	GLN	2.2
2	B5	622	LEU	2.2
10	L1	72	ASP	2.2
2	B3	449	PHE	2.2
13	P3	60	SER	2.2
1	A1	96	LYS	2.2
1	A1	326	LYS	2.2
10	L2	146	ASP	2.2
13	P2	62	GLN	2.2
1	A4	363	MET	2.2
1	A5	529	ILE	2.2
2	B5	237	ASP	2.2
2	B1	573	THR	2.2
5	E2	59	ASN	2.2
3	C1	17	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B2	544	ALA	2.2
3	C1	79	ALA	2.2
5	E4	42	LYS	2.2
6	F6	118	LEU	2.2
1	A1	192	ASN	2.2
1	A1	599	LEU	2.2
2	B1	583	TYR	2.2
4	D4	76	LYS	2.2
1	A2	288	VAL	2.2
6	F4	26	ALA	2.2
2	B1	514	LEU	2.1
6	F4	96	GLU	2.1
1	A2	46	THR	2.1
2	B5	465	PHE	2.1
13	P2	65	LEU	2.1
1	A3	508	THR	2.1
8	J2	14	LEU	2.1
13	P5	7	LEU	2.1
3	C4	39	ALA	2.1
5	E4	33	LYS	2.1
1	A2	32	GLY	2.1
1	A6	274	ALA	2.1
1	A6	156	PHE	2.1
1	A5	694	ARG	2.1
1	A5	18	ASN	2.1
1	A5	193	VAL	2.1
1	A2	119	PRO	2.1
1	A1	27	LYS	2.1
13	P3	1	ALA	2.1
1	A4	30	LYS	2.1
1	A6	96	LYS	2.1
4	D2	1	THR	2.1
1	A2	223	ILE	2.1
2	B4	253	ILE	2.1
8	J3	4	PHE	2.1
8	J4	15	ALA	2.1
13	P3	14	GLU	2.1
1	A2	115	GLN	2.1
6	F6	4	GLY	2.1
2	B6	515	PHE	2.1
8	J4	11	ALA	2.1
1	A5	748	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
13	P1	91	ASN	2.1
8	J1	39	HIS	2.1
12	X1	28	ALA	2.1
13	P4	62	GLN	2.1
13	P6	82	PRO	2.1
2	B6	295	GLY	2.1
1	A2	588	GLN	2.1
1	A3	150	SER	2.1
2	B1	293	GLN	2.1
4	D5	84	ARG	2.1
3	C6	21	PRO	2.1
1	A2	140	THR	2.1
1	A4	62	THR	2.1
1	A5	34	PHE	2.1
4	D5	24	GLU	2.1
1	A5	290	GLY	2.1
2	B6	253	ILE	2.1
12	X4	8	THR	2.1
4	D1	13	SER	2.1
1	A1	133	GLY	2.1
1	A1	85	ILE	2.1
10	L4	16	HIS	2.1
1	A3	278	PHE	2.1
1	A4	568	ASP	2.1
4	D1	59	ALA	2.1
13	P1	57	VAL	2.1
2	B6	478	ASP	2.1
1	A5	159	TYR	2.1
3	C6	67	TYR	2.1
1	A2	504	ASN	2.1
4	D6	3	LEU	2.1
4	D6	56	VAL	2.1
5	E6	23	VAL	2.1
1	A2	44	THR	2.1
1	A3	100	TYR	2.1
1	A4	57	ASP	2.1
13	P1	67	ASP	2.1
3	C1	58	PRO	2.1
5	E5	25	SER	2.1
6	F3	58	SER	2.1
5	E5	58	ASN	2.1
11	M2	31	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A2	383	LEU	2.0
1	A5	568	ASP	2.0
2	B1	480	LEU	2.0
3	C6	68	LEU	2.0
6	F1	1	ASP	2.0
2	B5	606	GLY	2.0
1	A2	478	THR	2.0
1	A3	694	ARG	2.0
2	B5	474	LEU	2.0
2	B4	477	PHE	2.0
4	D5	85	ILE	2.0
10	L2	22	SER	2.0
4	D1	55	LEU	2.0
2	B5	610	GLY	2.0
2	B5	517	THR	2.0
5	E4	55	VAL	2.0
10	L2	143	LEU	2.0
1	A1	695	GLY	2.0
1	A2	244	LEU	2.0
2	B6	292	THR	2.0
1	A6	145	GLN	2.0
4	D1	123	PRO	2.0
1	A1	296	ASP	2.0
1	A4	63	SER	2.0
5	E6	32	VAL	2.0
1	A1	34	PHE	2.0
10	L1	14	VAL	2.0
9	K3	55	GLY	2.0
10	L2	71	SER	2.0
13	P3	59	GLN	2.0
1	A3	728	ARG	2.0
2	B6	219	ALA	2.0
3	C2	29	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	CLA	A2	1601	45/65	-0.01	1.09	165,184,190,190	0
14	CLA	A4	853	45/65	0.20	1.13	169,176,185,190	0
14	CLA	A6	1601	45/65	0.28	1.05	164,174,180,182	0
16	BCR	B4	845	40/40	0.40	1.34	168,178,188,188	0
16	BCR	J1	104	40/40	0.45	1.08	163,174,179,182	0
16	BCR	B1	847	40/40	0.46	1.21	159,165,170,172	0
16	BCR	A6	1646	40/40	0.47	0.79	151,160,180,181	0
16	BCR	M4	101	40/40	0.48	0.69	150,158,166,167	0
14	CLA	B1	838	60/65	0.49	0.78	156,175,183,189	0
16	BCR	A4	844	40/40	0.49	0.95	169,175,180,181	0
16	BCR	B1	852	40/40	0.50	0.90	159,175,179,180	0
14	CLA	A1	809	45/65	0.50	0.53	162,179,183,186	0
16	BCR	A1	842	40/40	0.50	0.95	160,174,182,182	0
16	BCR	A1	847	40/40	0.50	1.17	150,163,176,179	0
16	BCR	J5	105	40/40	0.53	1.04	163,170,174,176	0
14	CLA	J1	101	45/65	0.54	0.69	171,180,185,187	0
16	BCR	B1	848	40/40	0.55	0.78	159,170,176,177	0
16	BCR	M3	1602	40/40	0.55	0.78	153,161,166,167	0
16	BCR	B4	849	40/40	0.56	1.60	151,166,173,174	0
14	CLA	A4	816	54/65	0.56	0.49	161,170,179,187	0
17	LHG	X3	101	23/49	0.57	0.39	157,168,180,181	0
16	BCR	B2	846	40/40	0.57	1.56	157,162,169,171	0
16	BCR	B1	844	40/40	0.58	0.78	154,166,184,185	0
16	BCR	B1	845	40/40	0.58	0.51	156,169,184,186	0
16	BCR	B5	1849	40/40	0.59	0.99	152,163,170,171	0
16	BCR	M5	101	40/40	0.59	0.54	150,159,163,165	0
14	CLA	B5	1839	60/65	0.59	0.93	153,164,172,189	0
15	PQN	B4	844	33/33	0.60	0.65	157,161,167,168	0
16	BCR	B6	847	40/40	0.60	1.42	161,169,172,173	0
16	BCR	A1	845	40/40	0.60	0.50	150,162,167,168	0
16	BCR	A1	846	40/40	0.60	0.80	156,168,177,178	0
14	CLA	A4	842	41/65	0.61	0.55	150,170,175,175	0
16	BCR	B2	845	25/40	0.61	0.98	154,165,177,178	0
16	BCR	B6	846	25/40	0.61	1.18	157,165,175,176	0
14	CLA	L5	202	45/65	0.61	0.81	167,179,181,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	BCR	A4	849	40/40	0.61	1.48	153,163,183,185	0
16	BCR	B3	1845	40/40	0.61	1.66	165,170,174,175	0
16	BCR	A4	847	40/40	0.61	0.65	159,169,176,177	0
15	PQN	A4	843	33/33	0.61	1.65	165,171,175,176	0
14	CLA	B1	821	47/65	0.61	0.50	155,179,183,190	0
16	BCR	B1	843	40/40	0.62	0.56	169,176,183,184	0
16	BCR	F1	1302	40/40	0.62	0.58	165,172,181,183	0
14	CLA	A1	815	49/65	0.62	0.60	150,175,181,185	0
15	PQN	A1	841	33/33	0.62	1.08	162,165,170,171	0
14	CLA	B1	834	58/65	0.63	0.58	159,174,184,186	0
16	BCR	L6	201	40/40	0.63	0.49	150,158,175,176	0
16	BCR	J4	104	40/40	0.64	1.14	163,169,174,176	0
17	LHG	B1	851	23/49	0.64	0.65	158,175,188,189	0
16	BCR	A4	848	40/40	0.64	0.79	160,168,174,174	0
16	BCR	J1	103	40/40	0.64	1.00	155,164,181,183	0
16	BCR	J5	104	40/40	0.64	1.24	150,161,168,169	0
19	LMG	B6	848	55/55	0.64	0.86	152,161,175,182	0
19	LMG	B5	1851	55/55	0.64	0.79	151,162,170,177	0
14	CLA	F1	1301	45/65	0.65	0.49	167,171,182,186	0
16	BCR	B6	844	40/40	0.65	0.98	156,172,183,183	0
16	BCR	M1	1202	40/40	0.65	0.48	150,161,172,174	0
14	CLA	L3	202	45/65	0.65	0.62	164,172,183,186	0
16	BCR	A1	843	40/40	0.65	0.93	163,171,178,180	0
17	LHG	X4	101	23/49	0.65	0.77	161,172,183,186	0
16	BCR	B5	1845	40/40	0.65	1.03	163,169,180,182	0
14	CLA	M3	1601	45/65	0.65	0.67	169,176,182,190	0
14	CLA	B1	818	59/65	0.66	0.83	160,171,185,190	0
19	LMG	B4	851	55/55	0.66	0.76	150,162,172,177	0
16	BCR	B5	1846	40/40	0.66	0.79	150,158,179,180	0
16	BCR	B1	849	40/40	0.66	0.61	158,169,173,174	0
16	BCR	A4	845	40/40	0.67	0.84	161,169,177,179	0
16	BCR	J6	1105	40/40	0.67	0.56	157,161,170,171	0
14	CLA	A1	811	54/65	0.67	0.48	153,160,169,171	0
16	BCR	B4	847	40/40	0.67	0.67	152,170,186,188	0
14	CLA	A1	823	59/65	0.67	0.34	153,162,170,173	0
16	BCR	B4	846	40/40	0.67	0.75	157,169,182,184	0
19	LMG	B1	850	55/55	0.67	0.79	156,167,178,183	0
16	BCR	A2	1648	40/40	0.67	0.58	159,169,174,175	0
14	CLA	A4	809	45/65	0.67	0.70	166,180,186,190	0
16	BCR	A6	1643	40/40	0.68	0.81	156,161,165,173	0
14	CLA	B6	831	49/65	0.68	0.51	150,164,173,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	BCR	F6	203	40/40	0.68	0.79	159,166,172,175	0
16	BCR	B6	843	40/40	0.68	0.80	159,167,170,171	0
15	PQN	B5	1844	33/33	0.68	0.57	152,161,167,170	0
14	CLA	B1	814	65/65	0.68	0.66	157,175,189,190	0
16	BCR	A4	846	40/40	0.68	0.82	157,168,174,175	0
14	CLA	B3	1821	65/65	0.68	1.02	163,174,178,186	0
16	BCR	A2	1650	40/40	0.68	0.63	157,163,170,173	0
16	BCR	A5	848	40/40	0.68	0.91	152,163,170,172	0
16	BCR	B3	1846	40/40	0.69	0.93	158,167,174,176	0
14	CLA	A1	804	65/65	0.69	0.62	153,166,172,174	0
16	BCR	B5	1848	25/40	0.69	1.40	150,159,167,169	0
16	BCR	B3	1848	25/40	0.69	0.91	164,169,177,178	0
17	LHG	A4	850	49/49	0.69	1.23	155,170,176,182	0
14	CLA	B5	1823	45/65	0.70	0.70	168,176,179,182	0
16	BCR	I4	101	40/40	0.70	0.51	150,154,168,173	0
16	BCR	A2	1647	40/40	0.70	0.62	153,160,173,174	0
14	CLA	A1	824	65/65	0.70	0.79	158,168,175,180	0
14	CLA	B4	838	45/65	0.70	0.40	161,171,175,178	0
16	BCR	F4	204	40/40	0.70	0.85	163,171,179,182	0
16	BCR	A1	844	40/40	0.70	0.81	157,169,182,183	0
16	BCR	A5	850	40/40	0.70	0.74	150,159,164,164	0
16	BCR	F4	201	40/40	0.70	0.96	161,169,176,177	0
16	BCR	B2	842	40/40	0.70	0.50	158,165,172,173	0
16	BCR	L1	209	40/40	0.70	0.46	150,153,169,170	0
14	CLA	B1	813	45/65	0.70	0.68	162,171,176,179	0
14	CLA	B5	1827	46/65	0.71	0.73	150,165,171,172	0
16	BCR	F4	203	40/40	0.71	0.89	161,166,178,179	0
16	BCR	A5	845	40/40	0.71	0.84	157,162,167,169	0
16	BCR	F3	203	40/40	0.71	1.01	155,165,170,171	0
14	CLA	B3	1824	55/65	0.71	0.43	151,163,167,170	0
16	BCR	J4	103	40/40	0.71	1.64	155,164,177,177	0
14	CLA	B1	835	45/65	0.71	0.64	154,178,181,184	0
17	LHG	A1	848	49/49	0.72	0.81	156,168,182,184	0
16	BCR	J2	103	40/40	0.72	1.11	160,164,169,171	0
14	CLA	F2	204	37/65	0.72	0.65	150,161,174,177	0
16	BCR	B2	843	40/40	0.72	0.76	154,164,176,177	0
16	BCR	B3	1847	40/40	0.72	0.57	151,160,175,176	0
14	CLA	A2	1618	49/65	0.73	0.57	150,175,185,189	0
14	CLA	B6	823	45/65	0.73	0.65	150,162,170,177	0
14	CLA	B1	826	46/65	0.73	0.57	150,169,179,181	0
14	CLA	A1	814	45/65	0.73	0.52	171,179,184,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	LHG	B2	849	23/49	0.73	0.27	154,164,173,174	0
14	CLA	J1	102	37/65	0.73	0.85	150,163,175,179	0
14	CLA	B1	812	45/65	0.73	0.39	155,169,175,177	0
14	CLA	A1	840	41/65	0.73	0.43	150,164,178,187	0
14	CLA	A4	815	49/65	0.73	0.48	166,176,184,188	0
14	CLA	F3	202	45/65	0.73	0.98	158,171,173,177	0
14	CLA	B1	831	45/65	0.73	0.40	154,167,171,175	0
17	LHG	A5	851	49/49	0.73	1.04	152,164,171,182	0
14	CLA	B1	840	47/65	0.73	0.41	150,171,176,179	0
14	CLA	B1	825	54/65	0.74	0.65	153,166,178,188	0
14	CLA	B1	802	65/65	0.74	0.73	155,170,178,186	0
14	CLA	A4	814	45/65	0.74	0.40	162,172,183,186	0
16	BCR	A3	850	40/40	0.74	0.59	150,158,164,164	0
14	CLA	A4	821	49/65	0.74	0.32	164,176,181,183	0
14	CLA	J5	101	45/65	0.74	0.49	156,172,176,176	0
14	CLA	A5	810	45/65	0.74	0.49	154,168,174,175	0
16	BCR	B4	848	25/40	0.74	1.17	160,164,169,171	0
14	CLA	B3	1826	54/65	0.74	1.27	152,160,171,175	0
14	CLA	B5	1822	47/65	0.74	0.59	150,168,175,177	0
16	BCR	L4	208	40/40	0.74	0.41	150,156,172,174	0
14	CLA	B4	824	55/65	0.74	0.56	158,171,177,177	0
16	BCR	B6	850	40/40	0.74	0.98	153,160,174,174	0
16	BCR	J5	103	40/40	0.74	0.74	152,160,167,170	0
16	BCR	A6	1645	40/40	0.74	0.82	152,163,171,173	0
14	CLA	B1	820	65/65	0.74	0.48	152,174,179,182	0
15	PQN	B3	1844	33/33	0.74	0.56	150,153,165,165	0
14	CLA	B1	827	65/65	0.74	0.78	150,166,179,182	0
14	CLA	A5	816	49/65	0.75	0.99	150,173,180,181	0
14	CLA	A4	824	65/65	0.75	0.69	161,170,177,181	0
16	BCR	M6	1202	40/40	0.75	0.53	152,161,166,167	0
16	BCR	B3	1849	40/40	0.75	1.37	154,160,173,174	0
14	CLA	B5	1817	45/65	0.75	0.41	150,159,179,183	0
14	CLA	B4	823	45/65	0.75	0.36	165,170,177,179	0
14	CLA	A4	825	65/65	0.75	0.69	151,160,173,177	0
14	CLA	B5	1819	59/65	0.75	0.60	156,164,169,173	0
14	CLA	A4	806	51/65	0.75	0.51	161,176,182,184	0
14	CLA	A1	822	51/65	0.75	0.30	160,169,175,176	0
14	CLA	A2	1615	60/65	0.75	0.65	152,162,169,170	0
16	BCR	A2	1649	40/40	0.75	0.58	150,164,171,171	0
14	CLA	A2	1645	41/65	0.75	0.51	150,164,172,174	0
14	CLA	B1	822	45/65	0.75	0.49	171,177,186,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	B5	1815	65/65	0.76	0.59	162,167,175,181	0
14	CLA	A1	820	65/65	0.76	0.41	153,161,173,179	0
14	CLA	A5	815	45/65	0.76	0.43	156,170,176,177	0
14	CLA	A1	803	59/65	0.76	0.67	150,159,176,180	0
14	CLA	B1	816	45/65	0.76	0.29	161,168,176,190	0
14	CLA	A1	837	51/65	0.76	0.57	157,169,178,185	0
16	BCR	A5	849	40/40	0.76	0.95	154,159,168,168	0
14	CLA	B4	811	65/65	0.76	0.50	150,158,174,177	0
14	CLA	B1	817	55/65	0.76	0.56	150,165,180,184	0
14	CLA	B5	1814	45/65	0.76	0.62	158,170,176,178	0
14	CLA	B2	829	45/65	0.76	0.47	151,163,171,172	0
16	BCR	A5	853	40/40	0.76	0.58	152,160,169,169	0
14	CLA	B1	805	65/65	0.76	0.77	153,170,176,180	0
16	BCR	B2	844	40/40	0.76	0.46	155,167,172,174	0
20	CA	L6	205	1/1	0.76	0.69	150,150,150,150	0
16	BCR	A6	1644	40/40	0.76	0.56	152,159,167,169	0
17	LHG	B6	849	23/49	0.76	0.41	155,169,180,180	0
14	CLA	K2	1401	45/65	0.76	0.39	161,170,176,177	0
19	LMG	B3	1850	55/55	0.76	0.85	157,163,172,176	0
14	CLA	B2	815	55/65	0.76	0.52	156,162,170,176	0
17	LHG	A2	1653	49/49	0.76	1.15	150,159,167,168	0
14	CLA	F4	202	45/65	0.77	0.57	161,174,177,179	0
16	BCR	B3	1851	40/40	0.77	0.93	150,164,176,177	0
14	CLA	B4	817	45/65	0.77	0.51	158,168,173,182	0
16	BCR	B5	1847	40/40	0.77	0.61	155,163,173,176	0
14	CLA	B2	814	45/65	0.77	0.38	159,165,174,176	0
14	CLA	B6	819	65/65	0.77	0.53	163,173,179,185	0
14	CLA	A4	804	65/65	0.77	0.66	156,164,173,174	0
14	CLA	J3	102	37/65	0.77	0.75	150,166,171,174	0
14	CLA	B1	823	55/65	0.77	0.46	167,173,179,188	0
16	BCR	F6	201	40/40	0.77	1.07	150,159,164,166	0
14	CLA	A3	809	65/65	0.77	0.71	150,162,168,175	0
14	CLA	B3	1817	45/65	0.77	0.45	154,168,182,190	0
14	CLA	L3	205	65/65	0.77	0.49	150,156,173,174	0
14	CLA	B4	809	65/65	0.77	0.48	150,157,167,173	0
14	CLA	B4	837	45/65	0.77	0.27	156,169,179,181	0
14	CLA	B1	824	45/65	0.77	0.56	160,164,170,175	0
14	CLA	B4	813	45/65	0.77	0.49	154,165,169,171	0
16	BCR	B6	845	40/40	0.77	0.82	150,168,174,176	0
14	CLA	A1	819	61/65	0.77	0.50	156,168,174,176	0
21	FES	P1	101	4/4	0.77	0.11	166,170,181,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	A2	1612	45/65	0.78	0.33	163,169,172,174	0
16	BCR	A3	849	40/40	0.78	0.86	150,158,166,168	0
14	CLA	A1	812	60/65	0.78	0.57	154,165,174,176	0
14	CLA	J4	101	45/65	0.78	0.76	162,176,181,183	0
16	BCR	L5	201	40/40	0.78	0.45	150,150,171,175	0
14	CLA	X3	102	45/65	0.78	0.64	161,167,171,174	0
14	CLA	K1	1401	45/65	0.78	0.41	161,173,177,179	0
16	BCR	F2	203	40/40	0.78	0.69	153,163,175,177	0
16	BCR	L3	201	40/40	0.78	0.43	150,154,161,162	0
14	CLA	A1	802	65/65	0.78	0.85	150,163,175,178	0
14	CLA	B2	818	65/65	0.78	0.65	155,169,174,177	0
16	BCR	A6	1648	40/40	0.78	1.12	150,158,169,170	0
15	PQN	A5	844	33/33	0.78	0.98	158,162,165,166	0
14	CLA	A1	805	65/65	0.78	0.62	156,171,178,182	0
14	CLA	B4	827	46/65	0.78	0.95	153,165,169,172	0
14	CLA	A4	834	45/65	0.78	0.33	156,166,171,181	0
14	CLA	B5	1818	55/65	0.78	0.73	153,161,181,183	0
14	CLA	F6	202	45/65	0.78	0.54	159,171,175,177	0
20	CA	L2	204	1/1	0.78	0.69	150,150,150,150	0
16	BCR	B1	846	25/40	0.78	1.32	166,173,175,176	0
14	CLA	B5	1821	65/65	0.78	0.58	152,168,175,180	0
17	LHG	X5	102	23/49	0.78	0.40	150,163,172,174	0
14	CLA	B3	1825	45/65	0.78	0.61	159,162,166,171	0
14	CLA	A1	821	49/65	0.78	0.36	164,175,180,182	0
14	CLA	A2	1607	65/65	0.78	0.74	150,155,167,170	0
14	CLA	A2	1627	65/65	0.78	0.66	155,163,170,176	0
14	CLA	A1	827	65/65	0.79	0.60	161,169,176,182	0
14	CLA	B5	1836	45/65	0.79	0.48	155,165,173,177	0
14	CLA	B3	1801	52/65	0.79	0.38	154,168,176,177	0
14	CLA	A6	1610	45/65	0.79	0.42	162,168,172,179	0
16	BCR	J3	104	40/40	0.79	0.92	151,158,164,165	0
16	BCR	J6	1104	40/40	0.79	1.13	150,156,161,161	0
14	CLA	B5	1813	45/65	0.79	0.45	151,170,178,181	0
16	BCR	I4	102	40/40	0.79	0.56	150,154,163,165	0
14	CLA	B1	853	52/65	0.79	0.43	150,160,171,175	0
16	BCR	A2	1652	40/40	0.79	0.98	150,159,167,167	0
14	CLA	B2	821	55/65	0.79	0.57	157,165,176,177	0
14	CLA	B1	801	65/65	0.79	0.45	150,160,166,169	0
14	CLA	A1	816	54/65	0.79	0.58	157,167,171,174	0
14	CLA	A6	1616	49/65	0.79	0.40	157,167,172,182	0
16	BCR	A5	846	40/40	0.79	1.05	150,162,174,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	CLA	B4	821	65/65	0.79	0.69	160,172,178,179	0
14	CLA	F5	1301	45/65	0.79	0.88	158,166,178,180	0
14	CLA	A2	1606	59/65	0.79	0.69	158,167,175,178	0
14	CLA	B1	803	65/65	0.79	0.34	150,164,171,175	0
14	CLA	A1	826	65/65	0.79	0.53	154,162,171,172	0
16	BCR	A3	847	40/40	0.79	0.82	150,159,167,171	0
16	BCR	I5	101	40/40	0.79	0.50	150,150,164,165	0
14	CLA	B6	816	55/65	0.79	0.57	150,162,172,178	0
14	CLA	K6	1401	45/65	0.79	0.32	159,163,170,173	0
19	LMG	B2	848	55/55	0.80	0.84	153,161,168,169	0
16	BCR	A5	847	40/40	0.80	0.95	150,159,163,163	0
14	CLA	B5	1801	52/65	0.80	0.49	162,171,177,185	0
16	BCR	L2	203	40/40	0.80	0.49	150,152,163,165	0
14	CLA	A2	1605	65/65	0.80	0.92	150,164,171,173	0
14	CLA	A1	836	47/65	0.80	0.36	151,166,173,174	0
14	CLA	B5	1832	45/65	0.80	0.64	158,166,173,177	0
14	CLA	A1	810	65/65	0.80	0.58	163,173,178,178	0
14	CLA	A1	833	45/65	0.80	0.49	158,171,178,180	0
16	BCR	F3	201	40/40	0.80	0.99	150,153,168,170	0
14	CLA	B1	832	49/65	0.80	0.46	151,161,177,183	0
14	CLA	B2	830	49/65	0.80	0.54	154,163,182,184	0
15	PQN	A2	1646	33/33	0.80	1.41	150,159,174,175	0
16	BCR	B2	850	40/40	0.80	0.62	160,165,168,169	0
14	CLA	B4	826	54/65	0.80	0.50	151,167,172,179	0
14	CLA	B4	819	59/65	0.80	0.35	156,168,178,185	0
14	CLA	X5	101	45/65	0.80	0.65	156,168,176,190	0
16	BCR	F2	201	40/40	0.80	0.96	154,162,168,169	0
16	BCR	B4	850	40/40	0.80	0.47	150,155,164,164	0
16	BCR	A2	1651	40/40	0.80	0.74	150,156,170,173	0
14	CLA	A6	1620	61/65	0.80	0.59	152,162,171,172	0
16	BCR	I2	101	40/40	0.80	0.46	150,150,161,162	0
14	CLA	B5	1838	45/65	0.80	0.59	159,168,175,181	0
14	CLA	B4	822	47/65	0.80	0.48	160,169,177,180	0
16	BCR	B5	1850	40/40	0.80	1.17	156,159,165,166	0
14	CLA	B5	1826	54/65	0.80	0.57	151,164,174,175	0
14	CLA	M2	1201	54/65	0.81	0.39	150,154,163,167	0
16	BCR	L1	203	40/40	0.81	0.54	150,152,158,160	0
16	BCR	A6	1647	40/40	0.81	0.73	152,159,166,167	0
14	CLA	K4	1401	45/65	0.81	0.33	162,170,175,185	0
14	CLA	B2	838	47/65	0.81	0.57	151,162,167,174	0
14	CLA	A1	838	65/65	0.81	0.82	154,165,172,176	0
14	CLA	B3	1828	65/65	0.81	0.65	150,162,175,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	B4	806	54/65	0.81	0.45	150,155,160,166	0
14	CLA	B5	1820	60/65	0.81	0.38	150,158,169,170	0
14	CLA	A2	1625	51/65	0.81	0.44	152,165,171,171	0
14	CLA	B3	1833	49/65	0.81	0.46	150,160,171,175	0
14	CLA	B4	839	60/65	0.81	0.62	162,168,172,173	0
14	CLA	X1	1701	45/65	0.81	0.39	169,175,181,182	0
16	BCR	J2	102	40/40	0.81	1.45	151,163,167,170	0
14	CLA	A3	810	45/65	0.81	0.51	152,162,166,173	0
14	CLA	A5	825	65/65	0.81	0.68	156,164,168,169	0
15	PQN	B6	842	33/33	0.81	0.58	153,163,168,175	0
14	CLA	B5	1824	55/65	0.81	0.51	163,168,179,181	0
16	BCR	A6	1652	40/40	0.81	0.57	150,151,158,163	0
14	CLA	B3	1823	45/65	0.81	0.64	157,165,175,179	0
14	CLA	B3	1838	45/65	0.81	0.46	157,168,174,179	0
14	CLA	A4	819	61/65	0.81	0.59	157,168,174,179	0
14	CLA	L6	202	65/65	0.81	0.55	150,150,166,168	0
16	BCR	I6	102	40/40	0.81	0.52	150,150,155,158	0
14	CLA	B1	837	45/65	0.81	0.27	157,167,179,183	0
14	CLA	A4	802	65/65	0.81	0.80	151,169,185,190	0
14	CLA	B4	852	52/65	0.81	0.36	150,163,170,172	0
14	CLA	A5	820	61/65	0.81	0.60	150,161,173,176	0
14	CLA	A3	823	51/65	0.81	0.44	152,164,176,182	0
14	CLA	A1	808	65/65	0.81	0.43	156,162,172,175	0
14	CLA	B1	807	65/65	0.82	0.44	155,168,179,187	0
14	CLA	B4	815	65/65	0.82	0.44	152,159,172,174	0
14	CLA	B2	822	45/65	0.82	0.50	156,162,173,175	0
16	BCR	F5	1302	40/40	0.82	0.86	152,162,178,180	0
14	CLA	A1	813	45/65	0.82	0.41	158,166,175,181	0
16	BCR	A3	851	40/40	0.82	0.64	150,152,168,173	0
14	CLA	L5	206	65/65	0.82	0.49	150,156,171,173	0
14	CLA	A4	803	59/65	0.82	0.46	160,166,175,179	0
14	CLA	A4	822	51/65	0.82	0.31	153,173,179,183	0
14	CLA	B1	836	45/65	0.82	0.36	160,169,173,178	0
14	CLA	A4	818	65/65	0.82	0.51	158,169,173,174	0
14	CLA	B6	826	65/65	0.82	0.81	155,165,174,178	0
14	CLA	B6	811	45/65	0.82	0.38	153,163,169,174	0
14	CLA	B3	1815	65/65	0.82	0.68	156,166,175,177	0
14	CLA	K5	101	41/65	0.82	0.32	150,161,167,169	0
14	CLA	A1	806	51/65	0.82	0.35	161,174,178,184	0
14	CLA	B1	808	65/65	0.82	0.50	150,166,178,183	0
14	CLA	B6	830	45/65	0.82	0.56	156,166,173,175	0
14	CLA	B5	1841	47/65	0.82	0.52	150,161,167,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	A6	1641	41/65	0.82	0.26	150,165,172,172	0
14	CLA	A2	1617	45/65	0.82	0.30	153,163,174,177	0
16	BCR	J3	103	40/40	0.82	0.80	150,158,164,165	0
14	CLA	B4	804	65/65	0.82	0.76	163,171,176,178	0
16	BCR	I1	102	40/40	0.82	0.43	150,156,162,169	0
14	CLA	A4	839	51/65	0.82	0.51	157,168,179,182	0
14	CLA	B4	841	47/65	0.82	0.79	161,174,179,179	0
14	CLA	J6	1102	45/65	0.82	0.37	159,166,174,178	0
14	CLA	A4	813	45/65	0.82	0.24	163,173,179,185	0
14	CLA	I1	101	65/65	0.82	0.53	150,151,162,166	0
14	CLA	B3	1822	47/65	0.82	0.67	160,172,175,176	0
14	CLA	B3	1837	45/65	0.82	0.31	155,168,174,178	0
14	CLA	B1	830	65/65	0.82	0.47	150,159,173,176	0
15	PQN	B1	842	33/33	0.82	0.58	154,161,168,173	0
14	CLA	B1	815	65/65	0.83	0.34	159,172,183,190	0
14	CLA	A2	1634	65/65	0.83	0.48	150,155,169,175	0
14	CLA	A1	828	65/65	0.83	0.67	154,161,169,175	0
14	CLA	A4	812	60/65	0.83	0.72	152,171,179,180	0
14	CLA	A4	817	54/65	0.83	0.36	159,164,171,173	0
14	CLA	B3	1832	45/65	0.83	0.29	153,164,178,189	0
14	CLA	M1	1201	54/65	0.83	0.43	155,166,175,180	0
14	CLA	B5	1830	65/65	0.83	0.65	154,162,168,170	0
14	CLA	B5	1835	58/65	0.83	0.71	150,168,175,176	0
14	CLA	B6	821	45/65	0.83	0.29	161,168,174,177	0
14	CLA	B5	1843	65/65	0.83	0.44	150,150,159,168	0
16	BCR	A3	848	40/40	0.83	0.78	150,158,161,163	0
14	CLA	B4	840	65/65	0.83	0.58	159,167,171,176	0
14	CLA	A6	1609	65/65	0.83	0.69	157,162,169,172	0
14	CLA	B2	824	46/65	0.83	0.70	150,161,167,169	0
14	CLA	A4	826	65/65	0.83	0.44	150,164,174,176	0
14	CLA	B3	1819	59/65	0.83	0.64	154,167,178,181	0
14	CLA	A3	816	49/65	0.83	0.54	150,168,179,186	0
14	CLA	A5	822	49/65	0.83	0.60	158,167,173,178	0
14	CLA	B4	808	65/65	0.83	0.51	154,165,174,179	0
16	BCR	A3	856	40/40	0.83	0.52	150,156,163,164	0
14	CLA	J2	101	45/65	0.83	0.65	160,171,177,178	0
14	CLA	B4	835	58/65	0.83	0.55	150,163,179,182	0
16	BCR	I3	101	40/40	0.83	0.53	150,150,161,162	0
14	CLA	B6	824	54/65	0.83	0.73	151,159,166,168	0
14	CLA	A5	828	65/65	0.83	0.46	150,163,173,178	0
20	CA	L4	207	1/1	0.83	0.58	150,150,150,150	0
14	CLA	A4	835	51/65	0.83	0.46	152,161,168,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	B4	830	65/65	0.84	0.48	150,166,171,174	0
14	CLA	B2	834	45/65	0.84	0.25	158,166,172,173	0
14	CLA	B6	820	47/65	0.84	0.47	157,173,176,178	0
14	CLA	B4	803	65/65	0.84	0.60	150,157,173,177	0
14	CLA	A6	1612	54/65	0.84	0.33	150,154,175,188	0
14	CLA	A3	807	51/65	0.84	0.61	157,165,169,177	0
14	CLA	B1	819	60/65	0.84	0.51	156,166,174,176	0
14	CLA	B3	1839	60/65	0.84	0.72	154,162,168,172	0
14	CLA	A6	1651	65/65	0.84	0.85	150,155,165,167	0
14	CLA	B1	839	65/65	0.84	0.27	160,167,172,183	0
14	CLA	B3	1816	65/65	0.84	0.42	159,165,173,180	0
14	CLA	A4	808	65/65	0.84	0.65	159,165,174,178	0
14	CLA	A6	1604	59/65	0.84	0.43	153,160,178,179	0
17	LHG	A2	1654	27/49	0.84	0.37	150,154,166,169	0
14	CLA	B3	1813	45/65	0.84	0.53	151,160,165,167	0
16	BCR	L2	201	40/40	0.84	0.39	150,151,160,163	0
14	CLA	A4	838	65/65	0.84	0.41	150,162,172,178	0
14	CLA	F2	202	45/65	0.84	0.40	150,174,180,184	0
14	CLA	L2	207	65/65	0.84	0.50	151,157,170,175	0
14	CLA	A1	818	65/65	0.84	0.78	159,166,175,178	0
14	CLA	B4	832	45/65	0.84	0.47	162,171,179,180	0
14	CLA	B4	818	55/65	0.84	0.36	155,164,172,174	0
14	CLA	B5	1831	65/65	0.84	0.70	150,154,173,175	0
14	CLA	B6	815	45/65	0.84	0.38	160,167,176,181	0
14	CLA	A2	1624	49/65	0.84	0.45	156,167,176,180	0
14	CLA	B6	840	65/65	0.84	0.45	150,151,165,169	0
14	CLA	B5	1828	65/65	0.84	0.53	150,158,166,168	0
16	BCR	L6	204	40/40	0.84	0.48	150,151,163,164	0
14	CLA	B5	1842	65/65	0.84	0.43	150,150,159,171	0
17	LHG	A3	853	49/49	0.84	0.91	150,154,165,168	0
14	CLA	K5	102	45/65	0.84	0.29	152,165,171,174	0
14	CLA	A5	837	65/65	0.84	0.38	151,160,168,173	0
14	CLA	B3	1820	60/65	0.84	0.70	150,159,166,166	0
14	CLA	K3	1401	45/65	0.84	0.28	150,163,168,173	0
14	CLA	B4	807	65/65	0.84	0.92	163,169,173,176	0
14	CLA	A5	843	52/65	0.84	0.39	160,166,175,177	0
14	CLA	A4	836	65/65	0.84	0.41	150,162,171,175	0
16	BCR	A3	852	40/40	0.84	0.84	150,156,159,160	0
14	CLA	A4	811	54/65	0.84	0.41	158,163,172,173	0
14	CLA	B5	1816	65/65	0.84	0.37	150,169,176,180	0
14	CLA	A2	1619	54/65	0.85	0.40	156,164,170,171	0
14	CLA	B3	1836	45/65	0.85	0.46	160,170,175,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	A4	830	50/65	0.85	0.50	150,164,172,173	0
14	CLA	L5	203	65/65	0.85	0.44	150,154,161,184	0
16	BCR	I1	103	40/40	0.85	0.81	150,152,167,169	0
14	CLA	B6	836	45/65	0.85	0.49	165,173,176,178	0
14	CLA	A2	1642	51/65	0.85	0.56	151,162,173,180	0
14	CLA	B4	820	60/65	0.85	0.43	150,160,169,171	0
14	CLA	A4	805	65/65	0.85	0.77	157,166,172,187	0
16	BCR	B2	847	40/40	0.85	0.49	150,150,158,161	0
14	CLA	B5	1809	65/65	0.85	0.45	150,154,160,166	0
14	CLA	A6	1638	47/65	0.85	0.48	150,156,166,170	0
14	CLA	B2	816	59/65	0.85	0.53	151,160,165,167	0
14	CLA	A6	1606	65/65	0.85	0.41	150,150,163,167	0
17	LHG	A6	1649	49/49	0.85	0.66	150,161,166,168	0
14	CLA	B5	1837	45/65	0.85	0.49	162,167,182,190	0
14	CLA	B2	810	45/65	0.85	0.43	150,155,163,169	0
14	CLA	A1	825	65/65	0.85	0.56	150,158,172,177	0
14	CLA	A2	1640	47/65	0.85	0.39	150,153,163,167	0
14	CLA	B6	812	45/65	0.85	0.34	157,169,173,177	0
14	CLA	A1	834	51/65	0.85	0.61	150,157,164,166	0
17	LHG	A1	849	27/49	0.85	0.21	162,166,171,172	0
14	CLA	B1	828	65/65	0.85	0.41	153,161,172,176	0
14	CLA	B4	814	45/65	0.85	0.26	162,168,176,178	0
14	CLA	A3	832	65/65	0.85	0.44	150,150,171,172	0
14	CLA	A3	802	65/65	0.85	0.49	150,153,161,165	0
14	CLA	A4	837	47/65	0.85	0.44	150,157,161,164	0
14	CLA	A5	804	59/65	0.85	0.68	150,155,167,178	0
14	CLA	B1	810	65/65	0.85	0.39	150,161,164,166	0
14	CLA	A3	820	61/65	0.85	0.82	150,154,168,171	0
14	CLA	A5	811	65/65	0.85	0.52	159,166,175,183	0
14	CLA	L1	207	65/65	0.85	0.41	150,155,163,167	0
14	CLA	B5	1833	49/65	0.85	0.79	150,156,168,175	0
14	CLA	B2	812	65/65	0.85	0.46	151,161,167,171	0
14	CLA	A6	1613	60/65	0.85	0.57	150,161,167,169	0
14	CLA	B2	835	45/65	0.85	0.40	156,171,176,179	0
14	CLA	B4	805	65/65	0.85	0.35	152,160,168,170	0
14	CLA	B4	802	65/65	0.86	0.60	158,170,177,177	0
14	CLA	B3	1809	65/65	0.86	0.47	150,157,170,180	0
14	CLA	A2	1623	65/65	0.86	0.60	150,159,164,170	0
14	CLA	A2	1641	65/65	0.86	0.57	150,161,172,173	0
14	CLA	A5	802	65/65	0.86	0.51	150,154,160,166	0
14	CLA	A2	1620	54/65	0.86	0.37	150,159,166,171	0
14	CLA	A5	832	65/65	0.86	0.38	150,150,164,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	CLA	A3	822	49/65	0.86	0.54	159,165,177,182	0
14	CLA	L6	208	65/65	0.86	0.53	150,157,166,168	0
14	CLA	A5	808	65/65	0.86	0.40	150,152,165,169	0
14	CLA	X4	102	45/65	0.86	0.40	165,175,181,182	0
14	CLA	L4	205	65/65	0.86	0.43	150,155,168,171	0
14	CLA	B4	816	65/65	0.86	0.34	150,162,167,169	0
14	CLA	B6	802	65/65	0.86	0.56	150,152,164,173	0
14	CLA	B6	817	59/65	0.86	0.60	163,168,173,175	0
14	CLA	J4	102	37/65	0.86	0.40	150,160,166,166	0
14	CLA	B3	1807	65/65	0.86	0.75	150,159,165,169	0
14	CLA	A3	824	59/65	0.86	0.47	150,150,167,173	0
14	CLA	M6	1201	54/65	0.86	0.43	150,160,165,168	0
14	CLA	B4	828	65/65	0.86	0.69	150,161,168,170	0
14	CLA	B5	1812	65/65	0.86	0.42	150,156,171,174	0
14	CLA	B3	1841	47/65	0.86	0.42	150,160,164,171	0
14	CLA	B3	1818	55/65	0.86	0.48	156,161,172,178	0
14	CLA	B6	839	47/65	0.86	0.49	151,158,170,173	0
14	CLA	B2	801	65/65	0.86	0.52	150,152,164,168	0
14	CLA	B3	1806	54/65	0.86	0.49	150,154,162,164	0
16	BCR	M2	1202	40/40	0.86	0.40	150,157,162,163	0
14	CLA	A3	844	41/65	0.86	0.42	150,159,167,173	0
14	CLA	B6	825	46/65	0.86	0.82	162,165,169,170	0
14	CLA	A6	1618	54/65	0.86	0.73	155,162,169,175	0
14	CLA	A4	831	65/65	0.86	0.36	150,156,171,172	0
14	CLA	A4	810	65/65	0.86	0.32	157,172,177,184	0
14	CLA	B6	806	65/65	0.86	0.65	150,161,171,173	0
14	CLA	A3	804	59/65	0.86	0.55	150,155,169,171	0
14	CLA	B5	1802	65/65	0.86	0.56	158,167,171,179	0
14	CLA	B1	829	65/65	0.86	0.59	159,171,175,177	0
14	CLA	B4	810	65/65	0.86	0.38	151,157,163,164	0
14	CLA	A4	829	65/65	0.86	0.70	152,165,168,169	0
14	CLA	L4	201	65/65	0.86	0.43	151,157,162,165	0
14	CLA	B5	1825	45/65	0.86	0.40	152,159,171,177	0
14	CLA	A3	817	54/65	0.86	0.59	150,156,161,164	0
14	CLA	A5	835	45/65	0.86	0.34	156,162,166,170	0
14	CLA	B5	1808	65/65	0.86	0.67	152,159,169,174	0
14	CLA	A2	1622	61/65	0.86	0.47	150,159,179,182	0
14	CLA	A5	840	51/65	0.86	0.81	156,161,172,182	0
14	CLA	A2	1611	65/65	0.86	0.68	154,162,168,174	0
14	CLA	B6	829	65/65	0.86	0.42	150,159,166,171	0
14	CLA	B5	1840	65/65	0.87	0.54	150,158,167,170	0
14	CLA	A1	835	65/65	0.87	0.42	150,163,168,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	A5	806	65/65	0.87	0.84	157,163,174,178	0
14	CLA	A6	1625	65/65	0.87	0.64	150,158,167,171	0
14	CLA	B2	819	47/65	0.87	0.51	162,165,175,176	0
16	BCR	L4	206	40/40	0.87	0.40	150,159,166,168	0
14	CLA	A3	845	52/65	0.87	0.30	156,160,169,177	0
14	CLA	A6	1623	51/65	0.87	0.54	160,165,174,180	0
14	CLA	B5	1804	65/65	0.87	0.45	154,161,165,168	0
14	CLA	B6	813	65/65	0.87	0.55	159,171,176,181	0
14	CLA	B5	1806	54/65	0.87	0.39	150,152,162,166	0
14	CLA	B1	809	65/65	0.87	0.35	150,156,173,174	0
14	CLA	J3	101	45/65	0.87	0.46	167,174,182,190	0
14	CLA	B1	806	65/65	0.87	0.35	150,156,162,168	0
14	CLA	A4	828	65/65	0.87	0.56	150,158,172,176	0
14	CLA	A5	836	51/65	0.87	0.56	150,150,158,163	0
14	CLA	B2	806	65/65	0.87	0.41	150,153,165,167	0
14	CLA	B4	812	65/65	0.87	0.46	150,154,166,168	0
14	CLA	B4	833	49/65	0.87	0.57	151,159,172,175	0
14	CLA	J6	1101	65/65	0.87	0.50	150,159,168,171	0
14	CLA	L6	203	65/65	0.87	0.45	150,150,162,167	0
14	CLA	A2	1638	51/65	0.87	0.43	150,150,157,165	0
14	CLA	A3	813	60/65	0.87	0.55	150,153,164,172	0
14	CLA	A5	803	65/65	0.87	0.62	150,156,175,176	0
14	CLA	A2	1632	65/65	0.87	0.70	150,157,162,163	0
14	CLA	B3	1835	58/65	0.87	0.49	153,162,174,176	0
14	CLA	A1	801	65/65	0.87	0.69	151,160,166,172	0
14	CLA	B2	840	65/65	0.87	0.39	150,152,159,164	0
16	BCR	L5	207	40/40	0.87	0.48	150,156,168,170	0
14	CLA	B6	818	60/65	0.87	0.61	150,159,169,172	0
14	CLA	L3	203	65/65	0.87	0.39	150,157,165,173	0
14	CLA	A2	1643	65/65	0.87	0.73	150,159,168,170	0
14	CLA	B4	801	65/65	0.87	0.42	150,159,164,171	0
14	CLA	A5	814	45/65	0.87	0.38	150,156,161,162	0
14	CLA	A1	807	65/65	0.87	0.45	150,158,169,172	0
14	CLA	B1	833	65/65	0.87	0.35	158,167,175,185	0
14	CLA	B4	842	65/65	0.87	0.41	150,154,165,168	0
16	BCR	L3	206	40/40	0.87	0.48	150,150,156,158	0
14	CLA	B5	1805	65/65	0.87	0.40	151,157,166,169	0
14	CLA	A1	829	65/65	0.87	0.66	158,167,171,172	0
14	CLA	A5	826	65/65	0.87	0.60	150,152,162,164	0
14	CLA	B6	814	65/65	0.87	0.51	150,162,179,188	0
14	CLA	A6	1617	54/65	0.88	0.54	150,156,163,165	0
14	CLA	X2	1701	45/65	0.88	0.40	162,170,173,177	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	L1	201	65/65	0.88	0.43	150,158,171,173	0
14	CLA	B1	804	65/65	0.88	0.70	153,161,175,177	0
14	CLA	B3	1842	65/65	0.88	0.41	150,150,160,166	0
15	PQN	B2	841	33/33	0.88	0.45	150,152,165,167	0
14	CLA	B6	809	65/65	0.88	0.46	150,155,163,170	0
14	CLA	B6	827	65/65	0.88	0.70	150,156,165,170	0
14	CLA	B5	1803	65/65	0.88	0.60	150,155,170,173	0
14	CLA	A3	805	65/65	0.88	0.69	150,150,167,170	0
14	CLA	B3	1830	65/65	0.88	0.43	150,156,165,171	0
14	CLA	B6	838	65/65	0.88	0.39	150,158,171,172	0
14	CLA	B4	825	45/65	0.88	0.35	152,162,168,174	0
14	CLA	A6	1626	65/65	0.88	0.49	150,150,161,163	0
14	CLA	A4	827	65/65	0.88	0.60	159,170,176,180	0
14	CLA	A3	815	45/65	0.88	0.57	158,167,169,174	0
14	CLA	B2	831	65/65	0.88	0.57	150,155,167,169	0
14	CLA	A5	813	60/65	0.88	0.49	150,159,167,168	0
15	PQN	A3	846	33/33	0.88	1.08	150,156,160,161	0
14	CLA	A2	1633	50/65	0.88	0.46	150,157,164,168	0
14	CLA	A5	830	65/65	0.88	0.65	150,159,165,169	0
14	CLA	B6	835	45/65	0.88	0.47	160,172,177,183	0
16	BCR	L6	209	40/40	0.88	0.50	150,153,163,167	0
14	CLA	B5	1807	65/65	0.88	0.70	152,160,170,178	0
14	CLA	B6	837	60/65	0.88	0.68	153,166,171,179	0
14	CLA	B4	843	65/65	0.88	0.40	150,154,166,169	0
14	CLA	A6	1615	45/65	0.88	0.60	150,161,166,169	0
14	CLA	A1	830	50/65	0.88	0.30	155,165,171,173	0
14	CLA	A1	817	54/65	0.88	0.53	151,161,168,169	0
14	CLA	B2	804	65/65	0.88	0.42	150,154,166,171	0
14	CLA	A3	818	54/65	0.88	0.62	150,153,159,163	0
14	CLA	J5	102	37/65	0.88	0.62	150,158,163,165	0
14	CLA	A4	823	59/65	0.88	0.42	150,162,176,184	0
14	CLA	L1	202	65/65	0.88	0.40	150,152,159,167	0
14	CLA	B5	1811	65/65	0.88	0.44	150,150,166,170	0
14	CLA	B3	1829	65/65	0.88	0.49	150,154,166,171	0
14	CLA	A5	807	51/65	0.88	0.34	156,163,167,175	0
14	CLA	B3	1814	45/65	0.88	0.30	159,168,173,180	0
14	CLA	A5	812	54/65	0.88	0.62	150,160,180,188	0
14	CLA	A2	1621	65/65	0.88	0.43	150,159,168,170	0
14	CLA	A3	812	54/65	0.88	0.57	150,155,174,178	0
14	CLA	A5	817	54/65	0.88	0.54	153,162,168,170	0
14	CLA	A3	825	65/65	0.88	0.67	150,157,165,171	0
14	CLA	B4	834	65/65	0.88	0.51	157,165,176,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	L1	206	65/65	0.88	0.41	150,153,165,169	0
14	CLA	L2	202	65/65	0.88	0.42	150,151,159,167	0
14	CLA	A5	838	47/65	0.88	0.49	150,158,165,168	0
14	CLA	A6	1635	45/65	0.88	0.26	150,156,162,166	0
14	CLA	A3	814	45/65	0.88	0.39	150,154,167,178	0
14	CLA	B3	1804	65/65	0.88	0.73	150,155,162,163	0
14	CLA	B6	833	58/65	0.88	0.66	150,155,176,180	0
14	CLA	B1	811	65/65	0.88	0.40	150,150,165,168	0
14	CLA	B3	1802	65/65	0.89	0.62	151,157,168,172	0
16	BCR	I3	102	40/40	0.89	0.48	150,152,159,165	0
14	CLA	B5	1829	65/65	0.89	0.63	150,156,169,170	0
14	CLA	A3	839	47/65	0.89	0.40	150,152,156,159	0
16	BCR	I5	102	40/40	0.89	0.47	150,150,169,171	0
14	CLA	A2	1613	65/65	0.89	0.59	151,161,170,174	0
14	CLA	B5	1834	65/65	0.89	0.59	154,160,168,169	0
14	CLA	A4	820	65/65	0.89	0.53	155,163,172,177	0
14	CLA	B6	805	65/65	0.89	0.45	150,154,161,163	0
14	CLA	B2	823	54/65	0.89	0.46	150,154,165,174	0
14	CLA	A6	1630	65/65	0.89	0.42	150,154,160,161	0
14	CLA	A3	826	65/65	0.89	0.46	150,150,165,169	0
14	CLA	B5	1810	65/65	0.89	0.43	150,150,169,176	0
14	CLA	A5	829	65/65	0.89	0.64	150,158,166,168	0
14	CLA	A2	1609	51/65	0.89	0.42	156,163,173,174	0
16	BCR	L2	208	40/40	0.89	0.44	150,150,161,165	0
14	CLA	B2	802	65/65	0.89	0.65	150,155,169,172	0
14	CLA	B2	833	45/65	0.89	0.49	150,165,171,173	0
14	CLA	A1	832	54/65	0.89	0.51	154,161,172,180	0
14	CLA	A5	805	65/65	0.89	0.63	150,162,170,172	0
14	CLA	B2	820	45/65	0.89	0.40	163,167,179,190	0
14	CLA	A2	1604	65/65	0.89	0.73	150,158,170,174	0
14	CLA	A4	807	65/65	0.89	0.68	151,162,174,175	0
14	CLA	A5	841	65/65	0.89	0.64	150,154,168,175	0
14	CLA	A2	1628	65/65	0.89	0.43	150,150,167,171	0
20	CA	L1	208	1/1	0.89	0.63	150,150,150,150	0
14	CLA	B6	832	65/65	0.89	0.57	150,158,173,175	0
14	CLA	A6	1607	51/65	0.89	0.34	157,163,166,168	0
14	CLA	A3	803	65/65	0.89	0.64	150,160,167,169	0
14	CLA	B6	807	65/65	0.89	0.49	151,159,166,168	0
14	CLA	B3	1834	65/65	0.89	0.66	152,159,168,170	0
14	CLA	A5	809	65/65	0.89	0.49	150,153,165,167	0
14	CLA	A2	1608	65/65	0.89	0.60	150,152,165,173	0
14	CLA	B2	827	65/65	0.89	0.42	150,156,164,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	L6	207	65/65	0.89	0.45	150,150,166,169	0
14	CLA	B2	839	65/65	0.89	0.38	150,154,163,167	0
14	CLA	A5	827	65/65	0.89	0.63	151,157,165,166	0
20	CA	L1	204	1/1	0.89	0.72	150,150,150,150	0
15	PQN	A6	1642	33/33	0.89	0.98	150,160,166,170	0
14	CLA	B4	831	65/65	0.89	0.48	150,153,168,172	0
14	CLA	J6	1103	37/65	0.89	0.29	150,157,165,166	0
14	CLA	A2	1629	65/65	0.89	0.46	150,158,169,174	0
14	CLA	A3	837	51/65	0.89	0.47	150,150,152,161	0
14	CLA	A6	1621	65/65	0.89	0.58	150,153,165,171	0
14	CLA	B2	803	65/65	0.89	0.42	150,153,157,160	0
14	CLA	A2	1637	45/65	0.89	0.31	152,156,167,173	0
14	CLA	A3	801	65/65	0.90	0.66	150,156,168,172	0
14	CLA	A2	1636	54/65	0.90	0.41	150,150,160,165	0
14	CLA	B3	1805	65/65	0.90	0.47	150,154,161,169	0
14	CLA	L5	204	65/65	0.90	0.40	150,159,167,172	0
14	CLA	A6	1640	65/65	0.90	0.71	150,155,170,178	0
14	CLA	B2	808	65/65	0.90	0.39	150,156,165,169	0
14	CLA	B2	825	65/65	0.90	0.66	150,155,168,177	0
14	CLA	B6	810	65/65	0.90	0.41	150,151,159,166	0
14	CLA	B2	813	65/65	0.90	0.41	155,160,169,173	0
14	CLA	A4	801	65/65	0.90	0.43	150,159,166,167	0
14	CLA	B2	826	65/65	0.90	0.43	150,156,167,170	0
14	CLA	B4	829	65/65	0.90	0.40	150,158,170,174	0
14	CLA	A3	811	65/65	0.90	0.51	152,163,169,173	0
14	CLA	A6	1633	65/65	0.90	0.40	150,155,163,172	0
14	CLA	A6	1627	65/65	0.90	0.55	150,156,175,176	0
14	CLA	A2	1626	59/65	0.90	0.52	150,152,165,167	0
14	CLA	A6	1639	51/65	0.90	0.48	150,155,165,173	0
14	CLA	B2	832	58/65	0.90	0.55	156,167,180,182	0
14	CLA	A2	1610	65/65	0.90	0.88	150,159,166,168	0
14	CLA	A3	827	65/65	0.90	0.60	150,150,166,167	0
14	CLA	A6	1603	65/65	0.90	0.65	151,159,173,176	0
14	CLA	A6	1611	65/65	0.90	0.43	156,161,167,170	0
14	CLA	A5	842	65/65	0.90	0.41	150,155,162,167	0
14	CLA	A6	1636	51/65	0.90	0.48	150,150,159,167	0
14	CLA	B2	809	65/65	0.90	0.43	150,154,162,168	0
14	CLA	B6	822	55/65	0.90	0.22	154,165,172,173	0
14	CLA	A4	833	54/65	0.90	0.32	150,157,168,169	0
14	CLA	B3	1843	65/65	0.90	0.41	150,150,154,156	0
14	CLA	A4	841	65/65	0.90	0.43	150,155,167,171	0
14	CLA	B3	1810	65/65	0.90	0.39	150,155,172,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	A3	819	65/65	0.90	0.64	150,156,166,176	0
14	CLA	A5	831	50/65	0.90	0.50	156,161,167,170	0
14	CLA	B2	836	60/65	0.90	0.51	154,159,166,168	0
14	CLA	A6	1619	65/65	0.90	0.64	150,159,169,176	0
14	CLA	L2	206	65/65	0.90	0.41	150,151,167,169	0
14	CLA	A4	832	65/65	0.90	0.38	150,154,162,163	0
14	CLA	B6	828	65/65	0.90	0.66	150,161,170,173	0
14	CLA	B2	811	45/65	0.90	0.28	150,160,169,175	0
14	CLA	B6	804	65/65	0.90	0.67	150,156,170,174	0
14	CLA	A3	831	50/65	0.91	0.50	150,155,163,168	0
17	LHG	A4	851	27/49	0.91	0.31	160,171,177,179	0
14	CLA	A3	821	65/65	0.91	0.60	150,150,160,171	0
14	CLA	A5	824	59/65	0.91	0.53	150,150,162,166	0
14	CLA	A6	1637	65/65	0.91	0.35	150,154,165,171	0
14	CLA	B6	841	65/65	0.91	0.38	150,150,156,162	0
14	CLA	A6	1622	49/65	0.91	0.35	160,167,175,177	0
14	CLA	A3	830	65/65	0.91	0.53	150,156,163,167	0
14	CLA	L3	204	65/65	0.91	0.41	150,150,164,166	0
14	CLA	A5	821	65/65	0.91	0.59	150,158,166,171	0
14	CLA	A2	1603	65/65	0.91	0.39	150,156,163,167	0
14	CLA	B4	836	45/65	0.91	0.26	150,165,171,173	0
14	CLA	A2	1614	54/65	0.91	0.26	151,156,168,171	0
14	CLA	A2	1635	65/65	0.91	0.42	150,152,157,160	0
14	CLA	B3	1811	65/65	0.91	0.44	150,151,166,167	0
14	CLA	A5	823	51/65	0.91	0.42	160,164,176,179	0
14	CLA	A5	839	65/65	0.91	0.64	154,159,167,175	0
14	CLA	B3	1827	46/65	0.91	0.51	150,164,170,172	0
14	CLA	B2	805	65/65	0.91	0.48	154,161,167,174	0
14	CLA	A2	1631	65/65	0.91	0.62	150,154,163,164	0
14	CLA	B6	803	65/65	0.91	0.69	157,163,168,173	0
14	CLA	A3	835	54/65	0.91	0.45	150,150,160,164	0
14	CLA	A3	841	51/65	0.91	0.60	150,154,165,175	0
14	CLA	A6	1629	65/65	0.91	0.50	150,150,158,159	0
14	CLA	B3	1812	65/65	0.91	0.43	150,151,160,163	0
14	CLA	L4	204	65/65	0.91	0.46	150,153,166,171	0
14	CLA	A6	1614	45/65	0.91	0.40	158,164,171,181	0
14	CLA	A3	840	65/65	0.91	0.86	154,163,170,175	0
14	CLA	B3	1803	65/65	0.91	0.71	150,152,164,165	0
14	CLA	B3	1840	65/65	0.91	0.60	151,158,170,173	0
14	CLA	B6	834	45/65	0.91	0.33	157,166,173,175	0
14	CLA	A4	840	65/65	0.91	0.65	150,157,171,175	0
14	CLA	A5	834	54/65	0.91	0.43	150,157,162,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	A2	1639	65/65	0.91	0.35	150,156,169,171	0
14	CLA	A2	1630	65/65	0.91	0.61	152,159,172,173	0
14	CLA	X6	1701	45/65	0.92	0.33	162,168,175,176	0
21	FES	P4	101	4/4	0.92	0.10	164,168,172,180	0
14	CLA	A6	1634	54/65	0.92	0.44	150,151,164,166	0
14	CLA	B6	808	65/65	0.92	0.45	150,156,166,173	0
14	CLA	A6	1608	65/65	0.92	0.59	150,155,161,162	0
14	CLA	B2	817	60/65	0.92	0.52	150,158,166,169	0
14	CLA	A2	1644	65/65	0.92	0.41	150,155,163,168	0
14	CLA	A3	829	65/65	0.92	0.45	150,150,157,161	0
14	CLA	B1	841	65/65	0.92	0.40	150,154,159,162	0
14	CLA	A3	836	45/65	0.92	0.32	153,162,167,172	0
14	CLA	A6	1631	50/65	0.92	0.51	150,155,161,166	0
17	LHG	A3	854	27/49	0.92	0.26	150,151,164,167	0
14	CLA	B2	828	65/65	0.92	0.58	150,159,168,169	0
14	CLA	A1	831	65/65	0.92	0.42	150,151,158,162	0
14	CLA	A3	828	65/65	0.92	0.52	150,157,167,171	0
17	LHG	A6	1650	27/49	0.92	0.32	150,157,163,170	0
14	CLA	I6	101	65/65	0.92	0.45	150,155,171,173	0
14	CLA	A5	833	65/65	0.92	0.46	150,150,154,160	0
14	CLA	A3	843	65/65	0.92	0.45	150,150,160,167	0
14	CLA	A1	839	65/65	0.92	0.47	150,152,159,163	0
14	CLA	A3	808	65/65	0.92	0.62	150,150,166,167	0
14	CLA	B2	837	65/65	0.92	0.39	150,159,167,169	0
14	CLA	A6	1632	65/65	0.92	0.42	150,150,156,160	0
14	CLA	L5	205	65/65	0.92	0.39	150,155,167,169	0
14	CLA	A6	1602	65/65	0.92	0.49	150,152,160,168	0
14	CLA	L2	205	65/65	0.92	0.39	150,158,163,166	0
18	SF4	C5	101	8/8	0.92	0.15	150,150,150,150	0
14	CLA	A6	1624	59/65	0.93	0.51	150,150,167,171	0
14	CLA	A6	1628	65/65	0.93	0.46	150,152,167,169	0
14	CLA	A3	842	65/65	0.93	0.59	150,155,162,163	0
14	CLA	A3	833	65/65	0.93	0.41	150,150,156,161	0
14	CLA	A2	1602	65/65	0.93	0.40	150,152,161,162	0
14	CLA	A2	1616	45/65	0.93	0.23	152,158,166,168	0
14	CLA	B1	854	65/65	0.93	0.39	150,151,165,174	0
17	LHG	A5	852	27/49	0.93	0.38	154,162,172,174	0
14	CLA	A6	1605	65/65	0.93	0.47	150,150,168,172	0
14	CLA	A3	806	65/65	0.93	0.46	150,157,163,169	0
18	SF4	C1	102	8/8	0.93	0.12	150,157,164,164	0
14	CLA	A5	818	54/65	0.93	0.41	150,155,165,168	0
14	CLA	B3	1808	65/65	0.93	0.63	150,160,168,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	B2	807	65/65	0.93	0.38	150,157,161,163	0
14	CLA	L4	203	65/65	0.93	0.42	150,150,169,171	0
14	CLA	A5	819	65/65	0.93	0.52	150,158,164,166	0
14	CLA	A3	838	65/65	0.94	0.36	150,156,165,167	0
20	CA	L4	202	1/1	0.94	0.61	150,150,150,150	0
14	CLA	A5	801	65/65	0.94	0.51	150,153,162,165	0
14	CLA	L6	206	65/65	0.94	0.38	150,155,167,174	0
14	CLA	B3	1831	65/65	0.94	0.50	150,156,168,173	0
14	CLA	L1	205	65/65	0.94	0.36	150,150,157,161	0
14	CLA	A3	834	65/65	0.94	0.42	150,156,166,169	0
18	SF4	C2	102	8/8	0.95	0.11	150,150,155,155	0
18	SF4	C1	101	8/8	0.95	0.12	150,150,150,153	0
18	SF4	A1	850	8/8	0.95	0.13	150,150,152,156	0
18	SF4	C5	102	8/8	0.95	0.10	150,150,154,154	0
18	SF4	C6	102	8/8	0.96	0.13	150,150,150,150	0
18	SF4	C6	101	8/8	0.96	0.15	150,150,150,150	0
18	SF4	A2	1655	8/8	0.96	0.18	150,150,150,150	0
18	SF4	A4	852	8/8	0.96	0.10	150,150,152,153	0
21	FES	P6	101	4/4	0.96	0.16	155,158,163,170	0
18	SF4	A5	854	8/8	0.96	0.15	150,150,150,150	0
21	FES	P2	101	4/4	0.96	0.10	160,160,163,168	0
18	SF4	C4	101	8/8	0.97	0.12	150,150,150,151	0
21	FES	P3	101	4/4	0.97	0.12	150,150,150,150	0
18	SF4	C2	101	8/8	0.97	0.17	150,150,150,150	0
18	SF4	C4	102	8/8	0.97	0.08	150,150,159,159	0
21	FES	P5	101	4/4	0.98	0.12	161,161,167,168	0
18	SF4	B6	801	8/8	0.98	0.17	150,150,150,150	0
18	SF4	C3	102	8/8	0.98	0.17	150,150,150,150	0
18	SF4	C3	101	8/8	0.98	0.18	150,150,150,150	0
18	SF4	A3	855	8/8	0.98	0.20	150,150,150,150	0

6.5 Other polymers ⓘ

There are no such residues in this entry.