



# wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

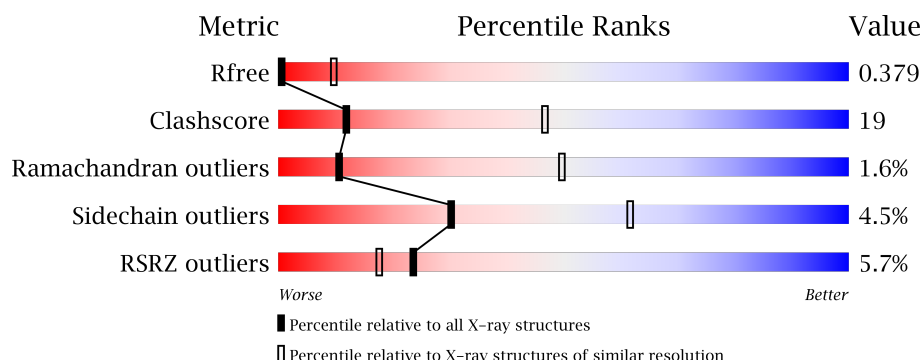
# 1 Overall quality at a glance

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  $\geq 3$ , 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.

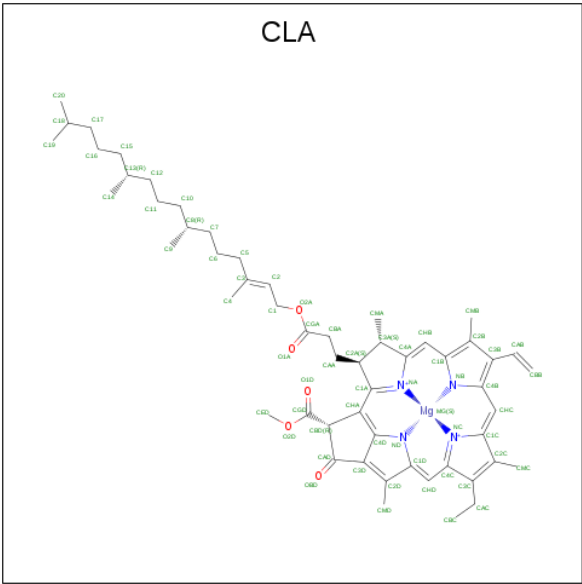
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P1	97	Total	C	N	O	S	0	0	0
			748	463	116	164	5			
13	P2	97	Total	C	N	O	S	0	0	0
			748	463	116	164	5			

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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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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

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

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

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

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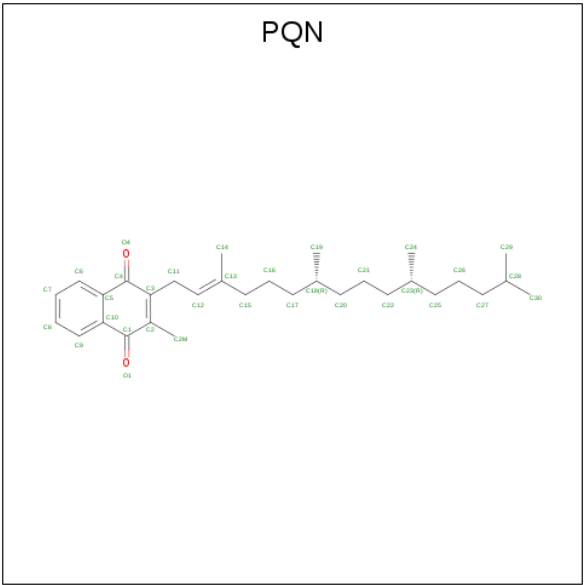
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B5	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	B5	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
14	B5	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	B5	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
14	B5	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	B5	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	B5	1	Total 45	C 35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

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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: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



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		

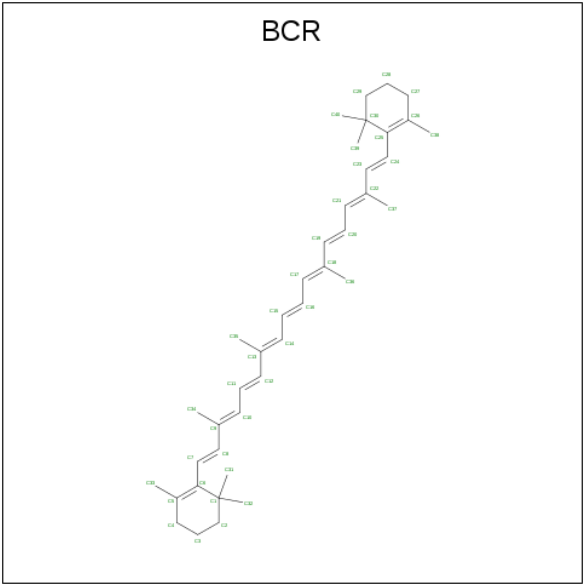
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B6	1	Total	C	O	0	0
			33	31	2		
15	A5	1	Total	C	O	0	0
			33	31	2		
15	B5	1	Total	C	O	0	0
			33	31	2		

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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	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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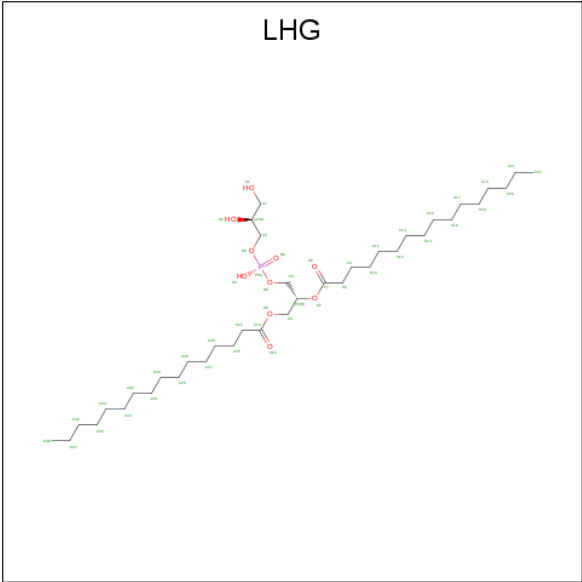
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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16	A6	1	Total C 40 40	0	0
16	A6	1	Total C 40 40	0	0
16	B6	1	Total C 40 40	0	0
16	B6	1	Total C 40 40	0	0
16	B6	1	Total C 40 40	0	0
16	B6	1	Total C 25 25	0	0
16	B6	1	Total C 40 40	0	0
16	B6	1	Total C 40 40	0	0
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: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



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		

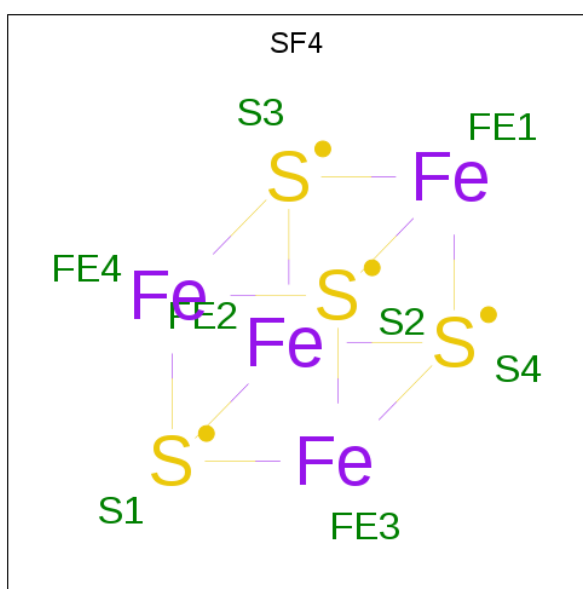
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B6	1	Total	C	O	P	0	0
			23	12	10	1		
17	A5	1	Total	C	O	P	0	0
			49	38	10	1		
17	A5	1	Total	C	O	P	0	0
			27	16	10	1		
17	X5	1	Total	C	O	P	0	0
			23	12	10	1		

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



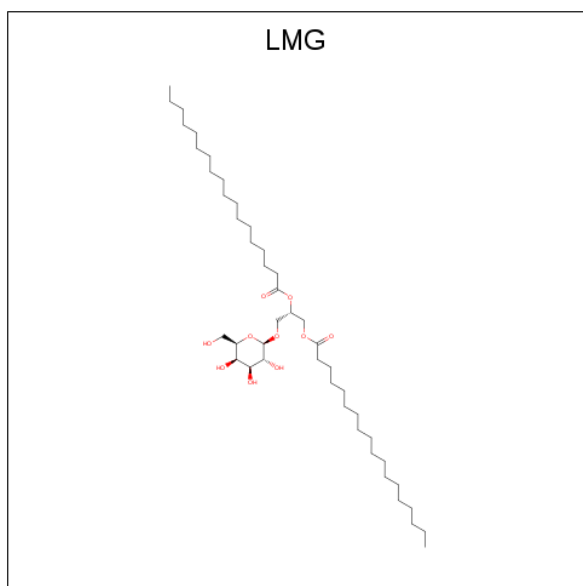
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A1	1	Total	Fe	S	0	0
			8	4	4		
18	C1	1	Total	Fe	S	0	0
			8	4	4		
18	C1	1	Total	Fe	S	0	0
			8	4	4		
18	A2	1	Total	Fe	S	0	0
			8	4	4		
18	C2	1	Total	Fe	S	0	0
			8	4	4		
18	C2	1	Total	Fe	S	0	0
			8	4	4		
18	A3	1	Total	Fe	S	0	0
			8	4	4		

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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:  $C_{45}H_{86}O_{10}$ ).

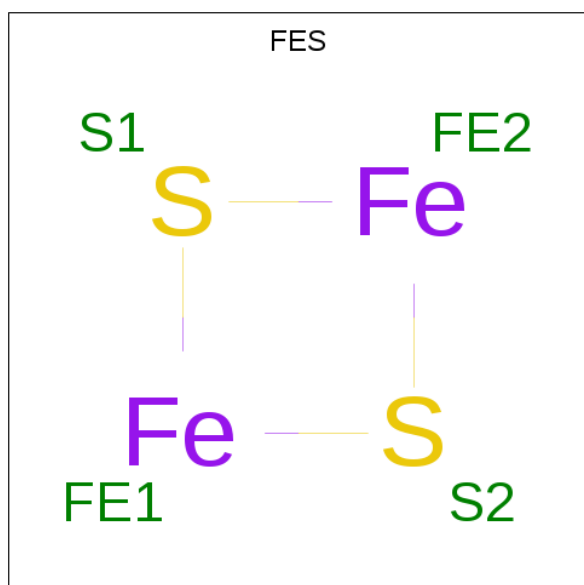


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	B1	1	Total C O 55 45 10	0	0
19	B2	1	Total C O 55 45 10	0	0
19	B3	1	Total C O 55 45 10	0	0
19	B4	1	Total C O 55 45 10	0	0
19	B6	1	Total C O 55 45 10	0	0
19	B5	1	Total C O 55 45 10	0	0

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

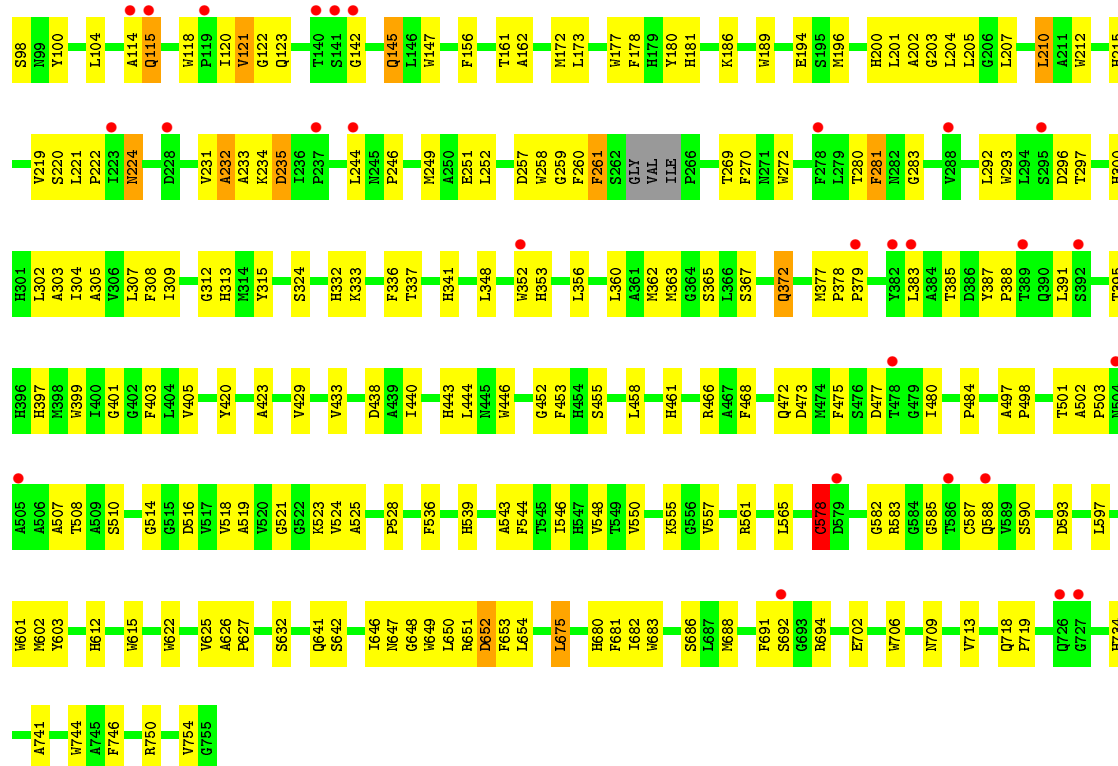
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	L6	1	Total Ca 1 1	0	0
20	L4	2	Total Ca 2 2	0	0
20	L1	2	Total Ca 2 2	0	0
20	L2	1	Total Ca 1 1	0	0

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

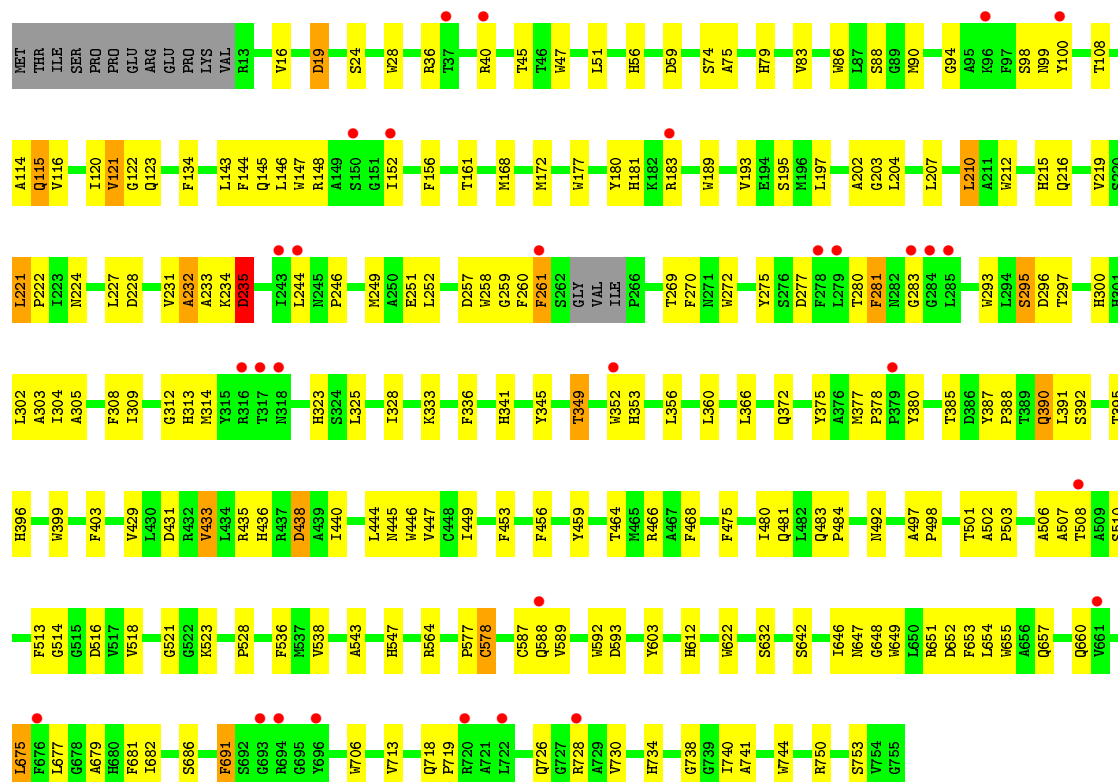


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	P1	1	Total 4	Fe 2	S 2	0	0
21	P2	1	Total 4	Fe 2	S 2	0	0
21	P3	1	Total 4	Fe 2	S 2	0	0
21	P4	1	Total 4	Fe 2	S 2	0	0
21	P6	1	Total 4	Fe 2	S 2	0	0
21	P5	1	Total 4	Fe 2	S 2	0	0

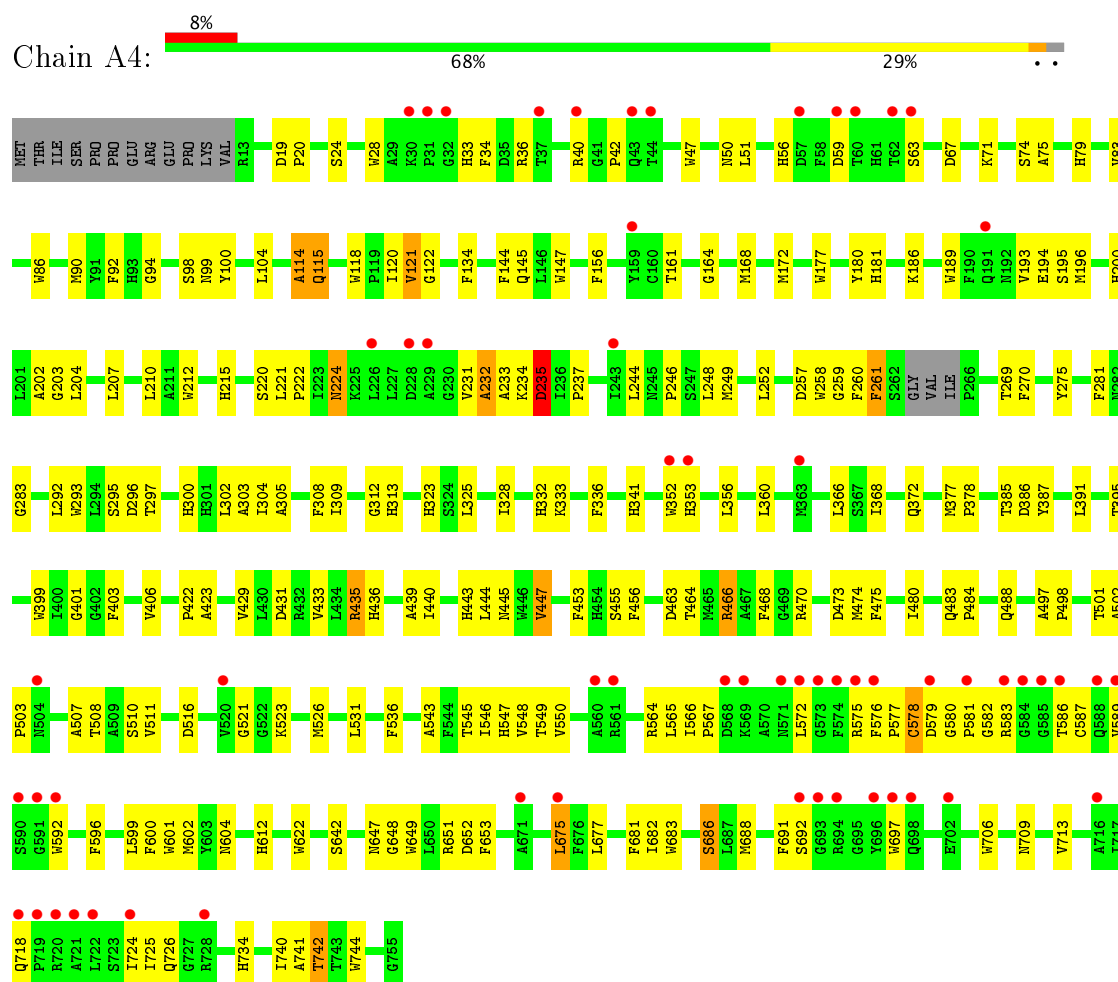




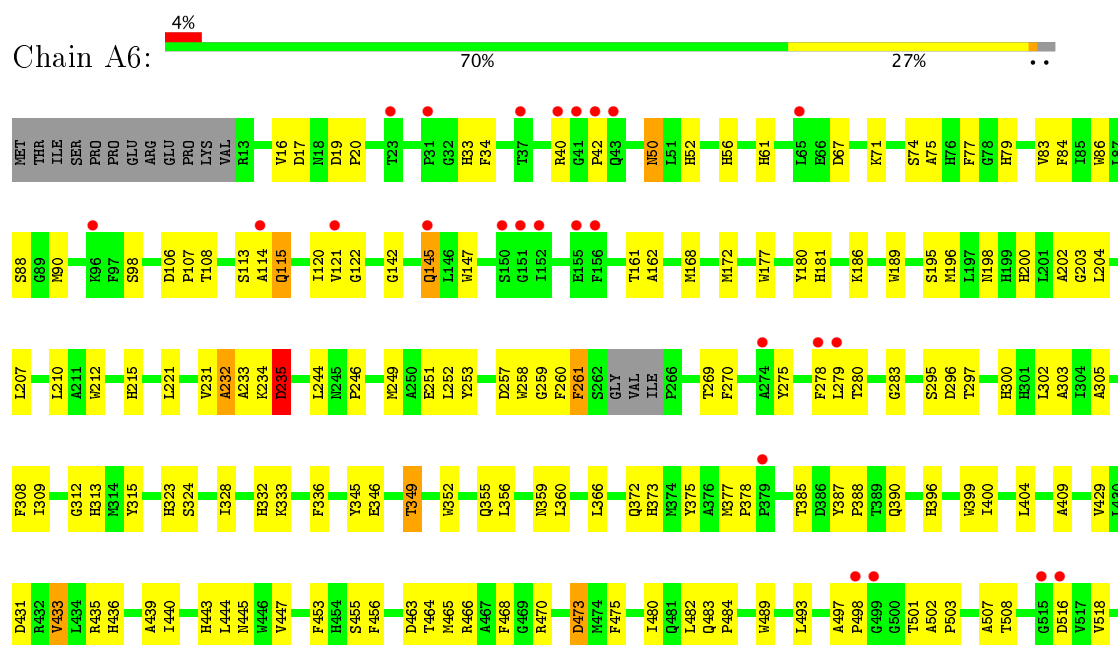
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

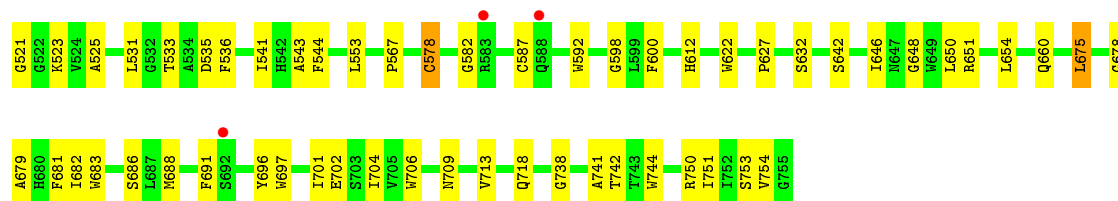


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

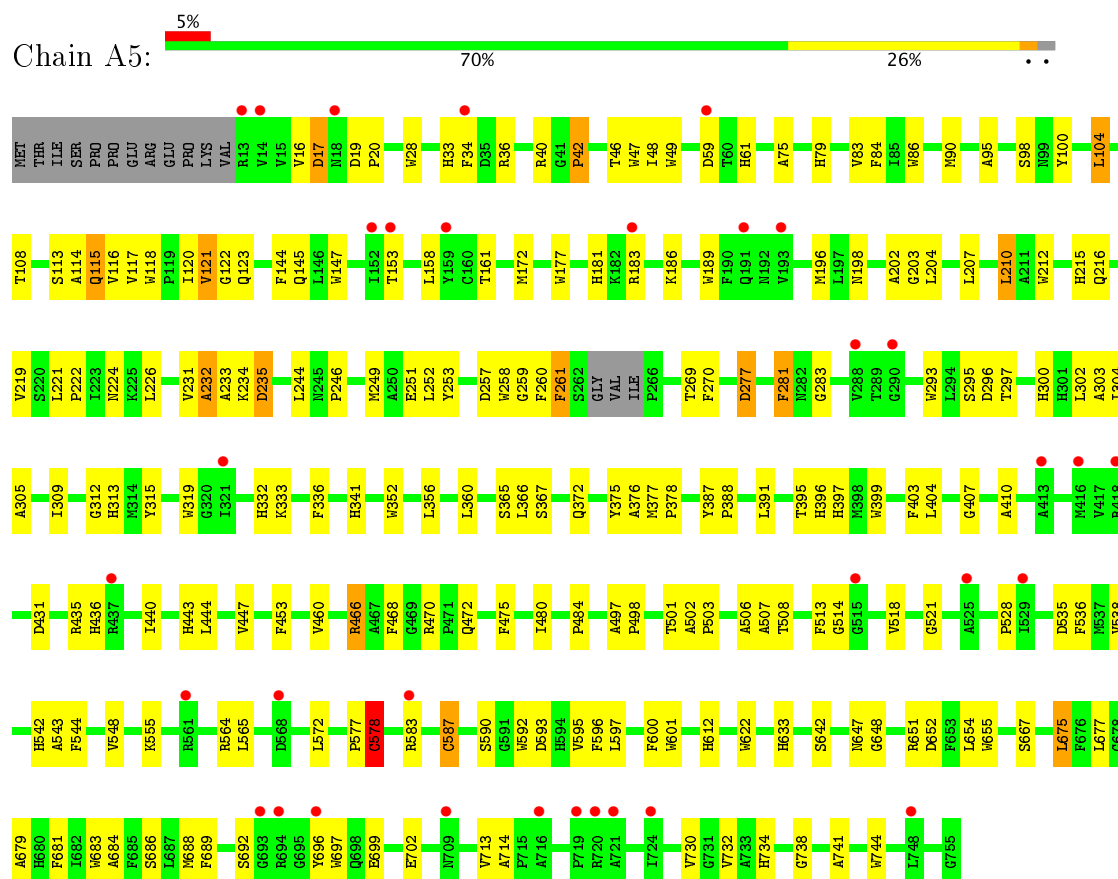


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

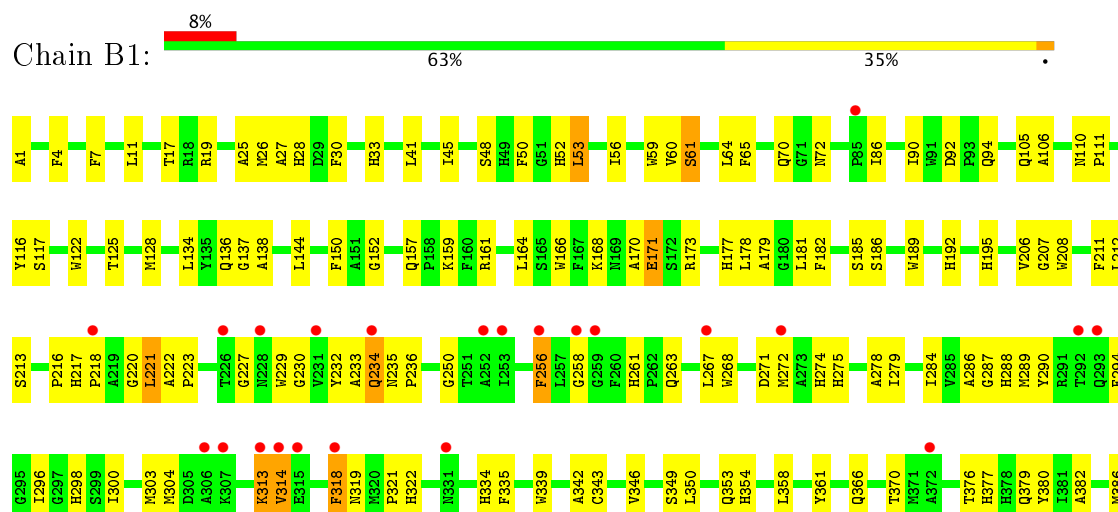




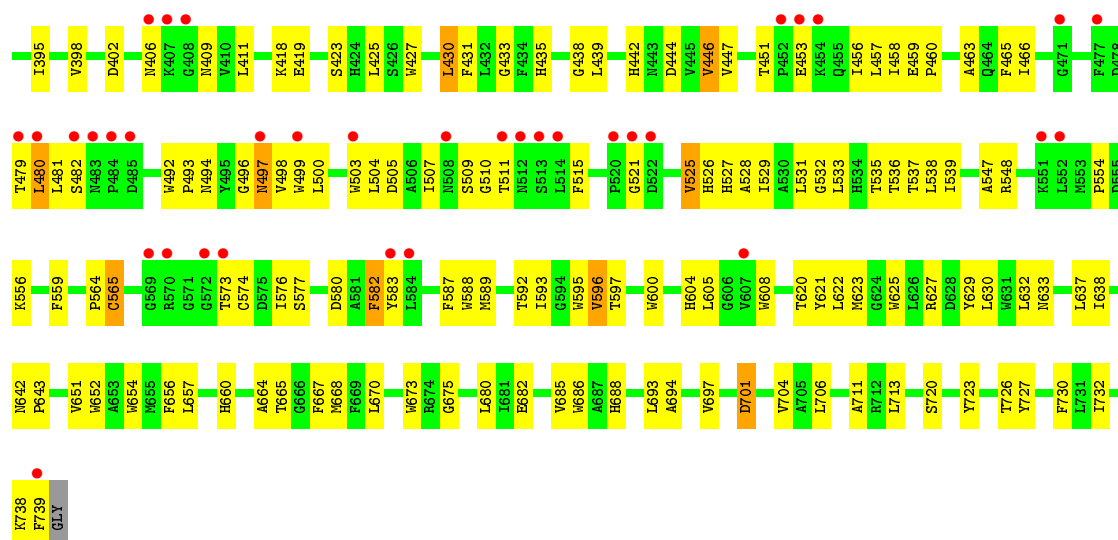
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



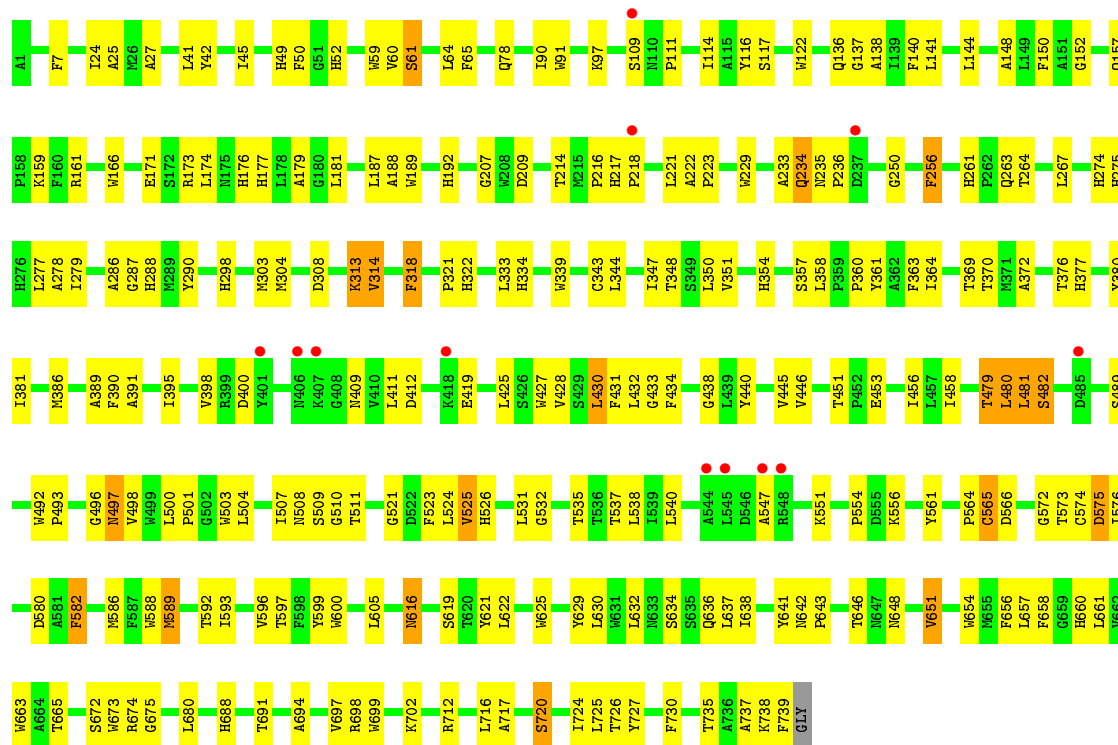
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





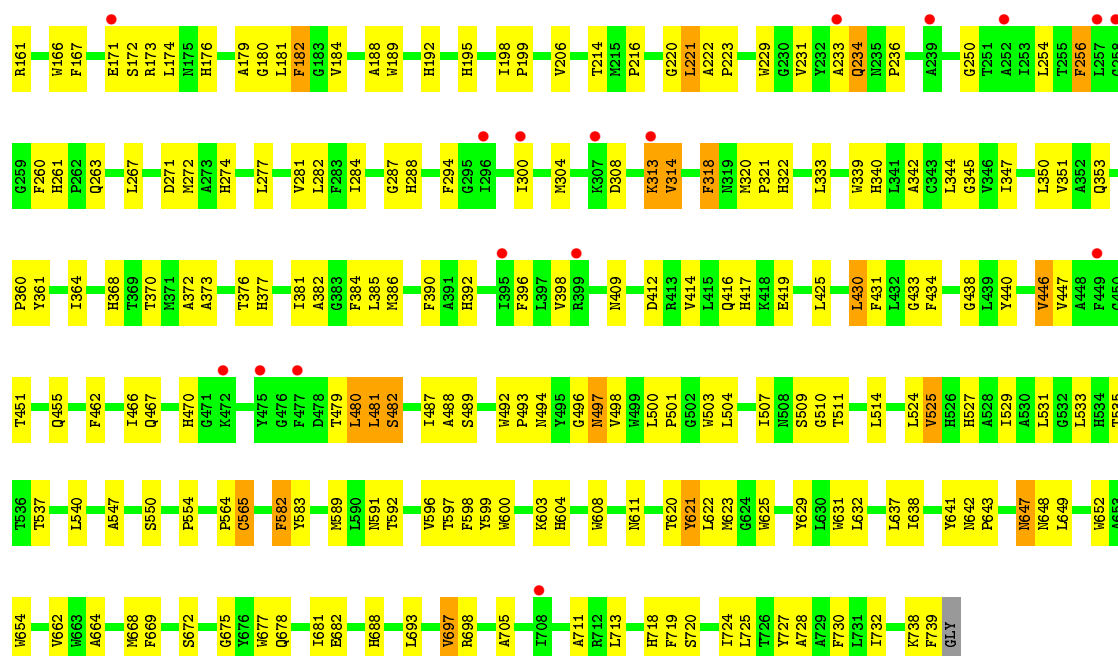


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

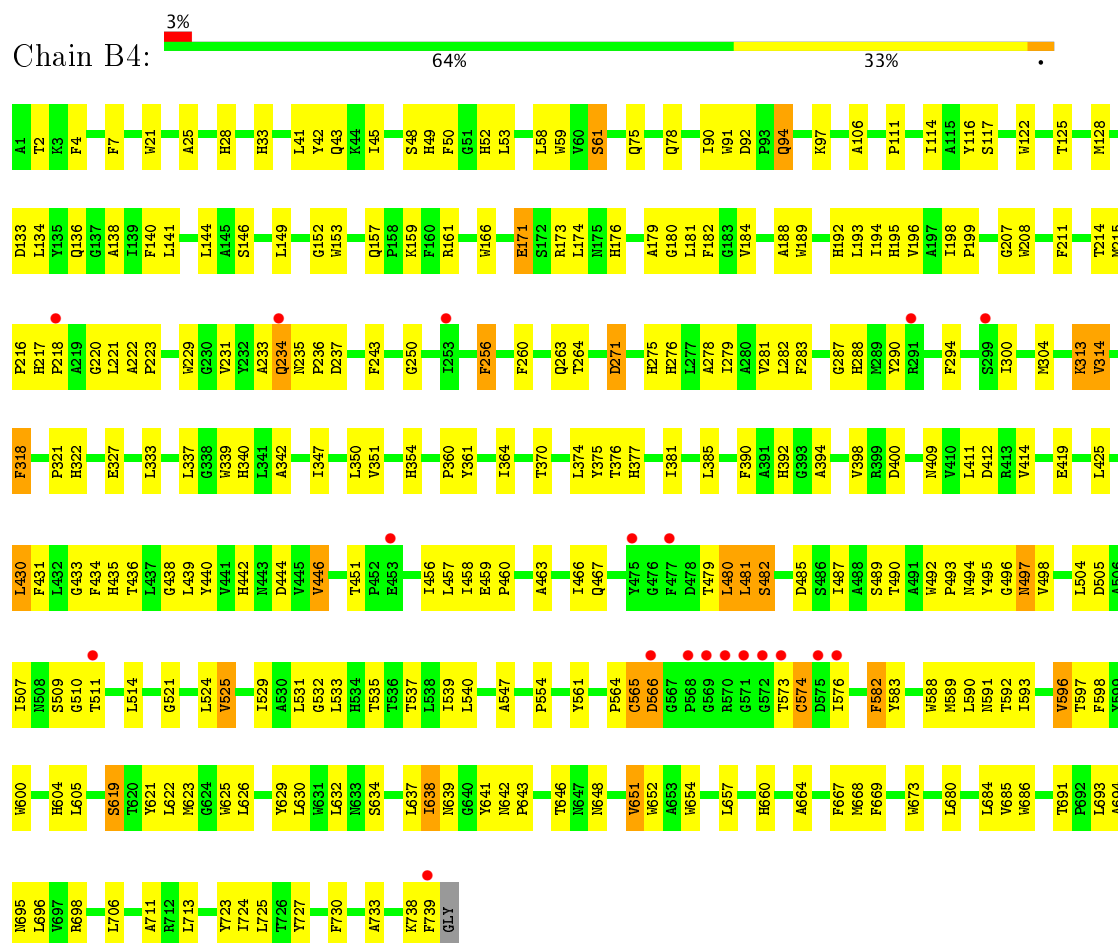


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

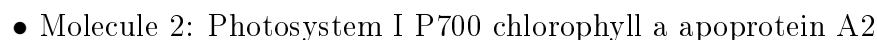




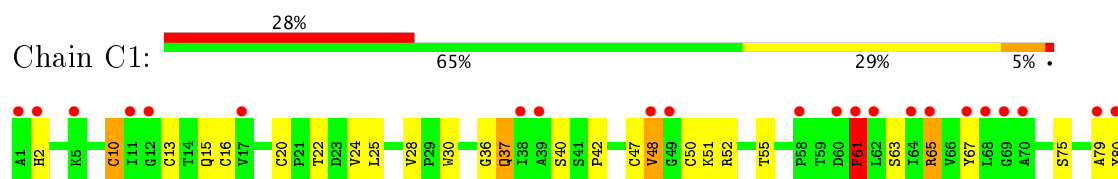
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



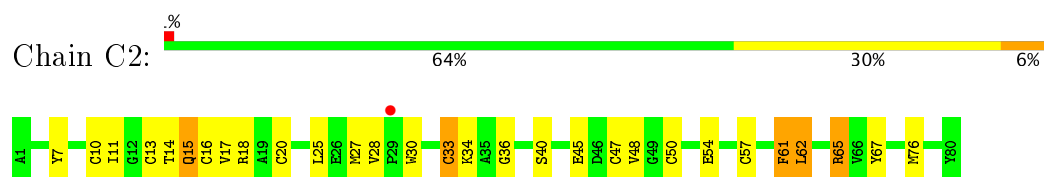
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



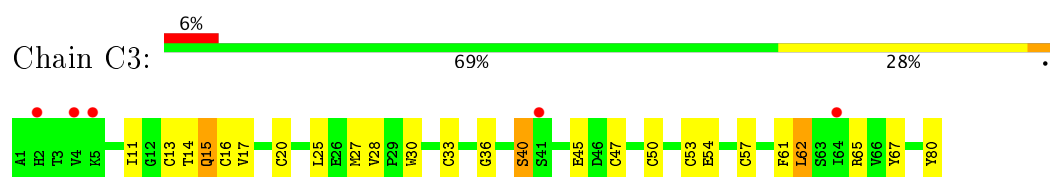
- Molecule 3: Photosystem I iron-sulfur center



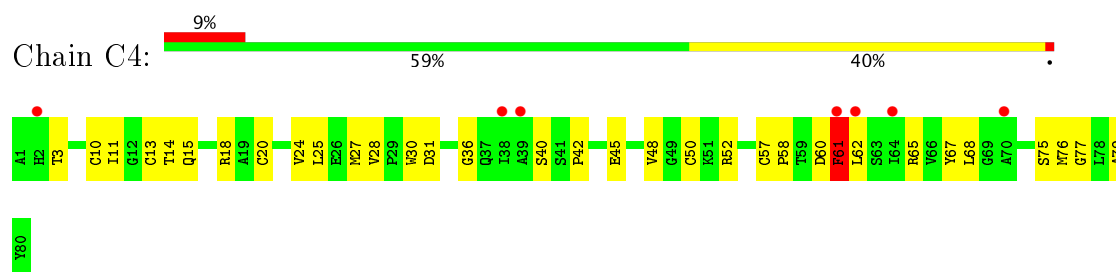
- Molecule 3: Photosystem I iron-sulfur center



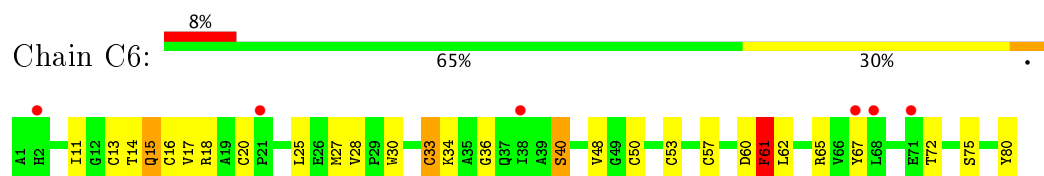
- Molecule 3: Photosystem I iron-sulfur center



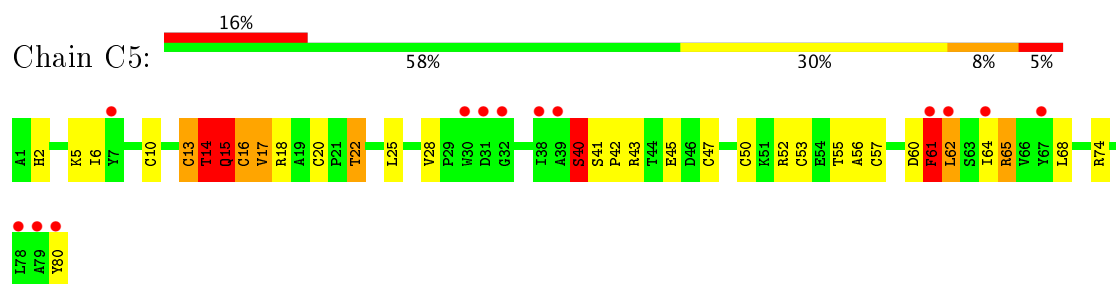
- Molecule 3: Photosystem I iron-sulfur center



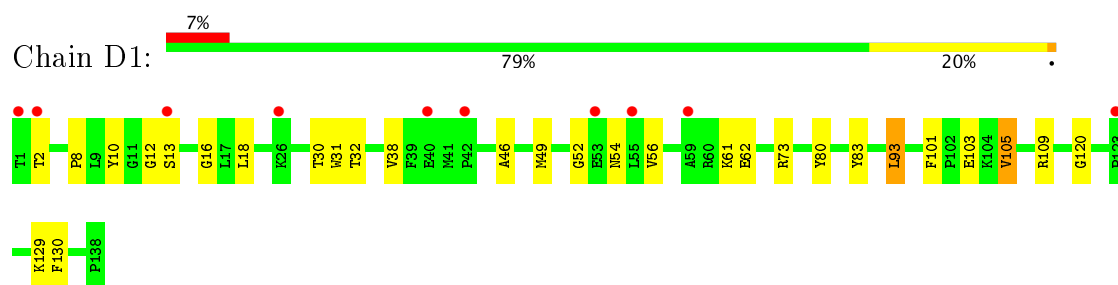
- Molecule 3: Photosystem I iron-sulfur center



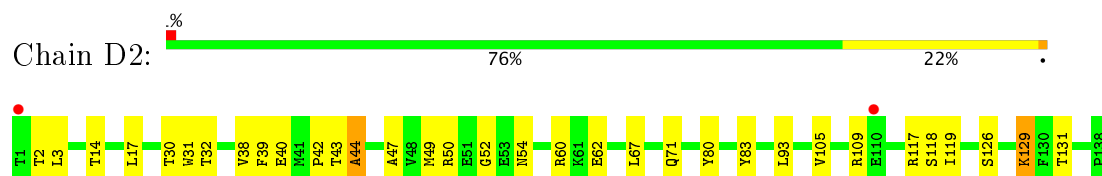
- Molecule 3: Photosystem I iron-sulfur center



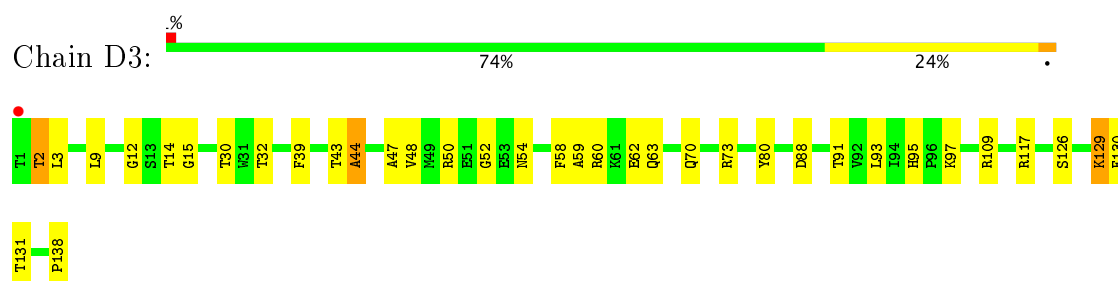
- Molecule 4: Photosystem I reaction center subunit II



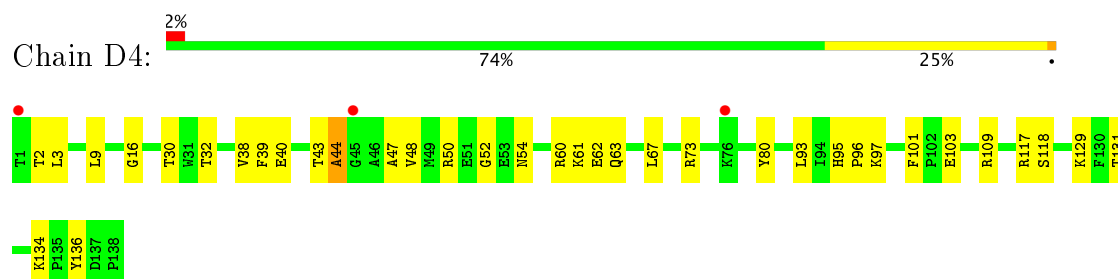
- Molecule 4: Photosystem I reaction center subunit II



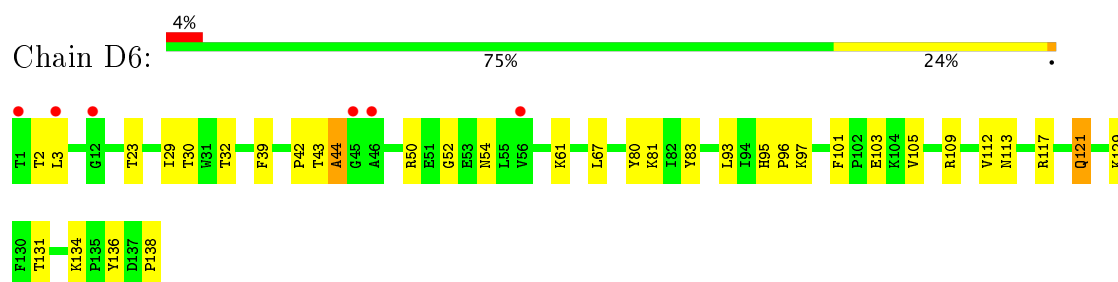
- Molecule 4: Photosystem I reaction center subunit II



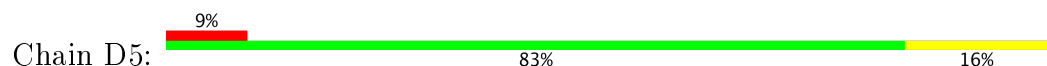
- Molecule 4: Photosystem I reaction center subunit II

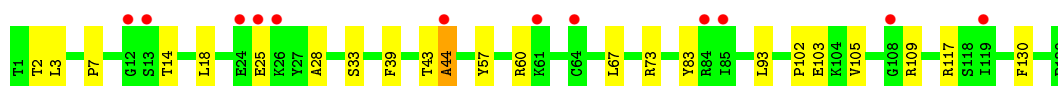


- Molecule 4: Photosystem I reaction center subunit II

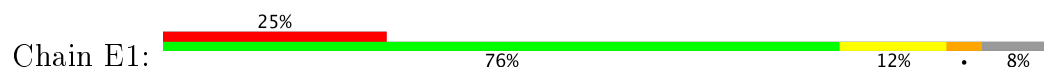


- Molecule 4: Photosystem I reaction center subunit II

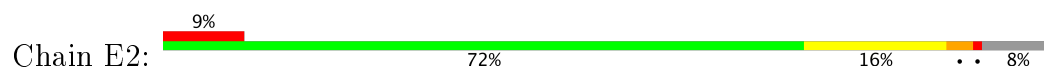




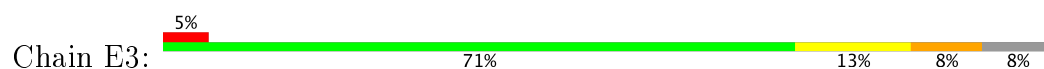
• Molecule 5: Photosystem I reaction center subunit IV



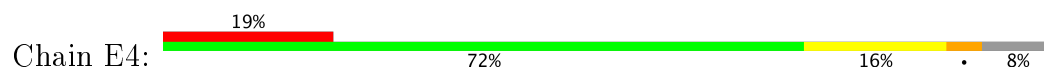
• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 5: Photosystem I reaction center subunit IV



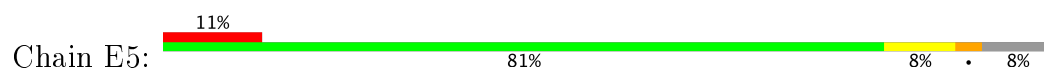
• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 5: Photosystem I reaction center subunit IV

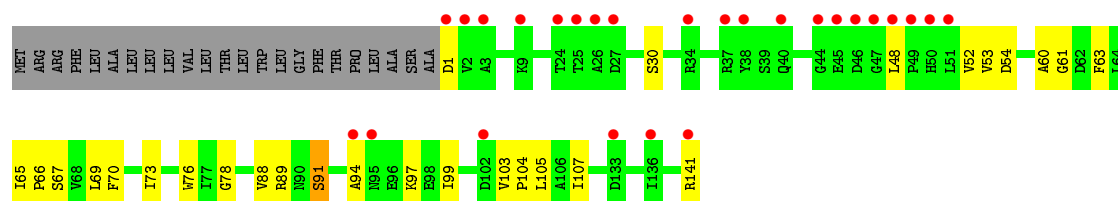


• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III

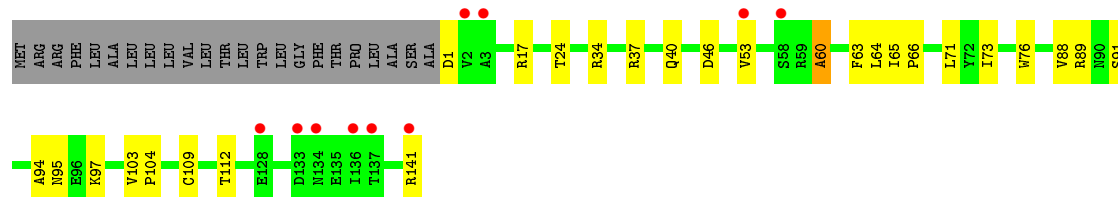




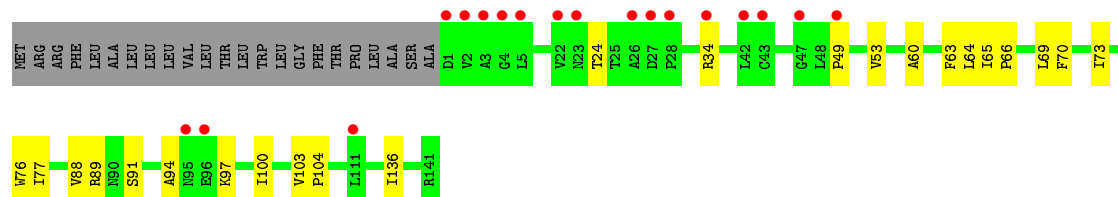
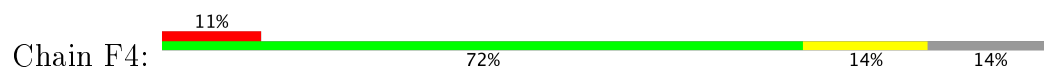
• Molecule 6: Photosystem I reaction center subunit III



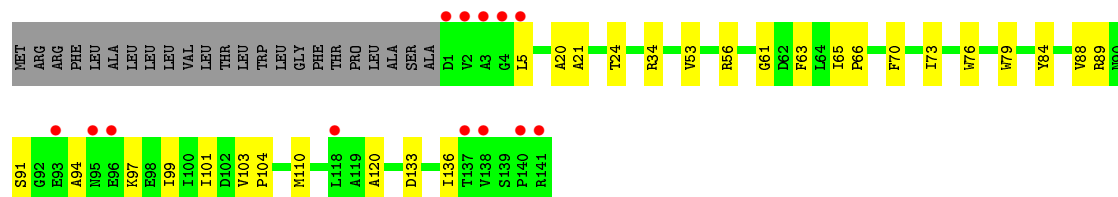
• Molecule 6: Photosystem I reaction center subunit III



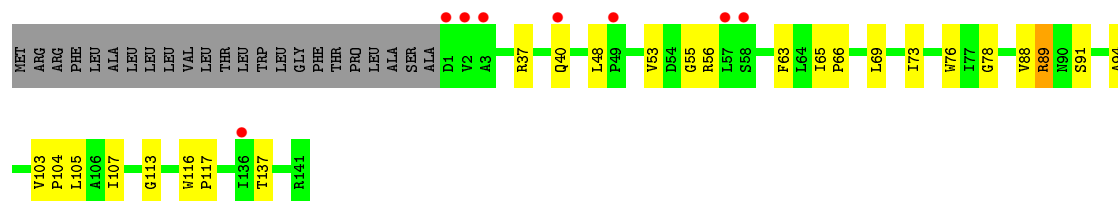
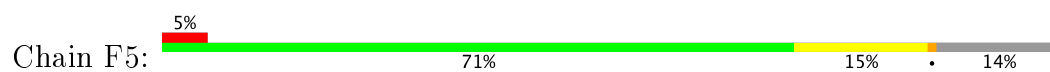
• Molecule 6: Photosystem I reaction center subunit III



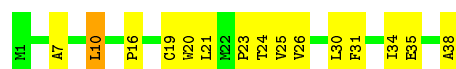
• Molecule 6: Photosystem I reaction center subunit III



• Molecule 6: Photosystem I reaction center subunit III



- Molecule 7: Photosystem I reaction center subunit VIII



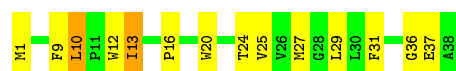
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 7: Photosystem I reaction center subunit VIII



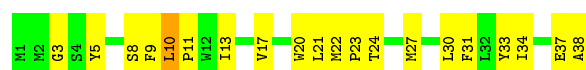
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 7: Photosystem I reaction center subunit VIII

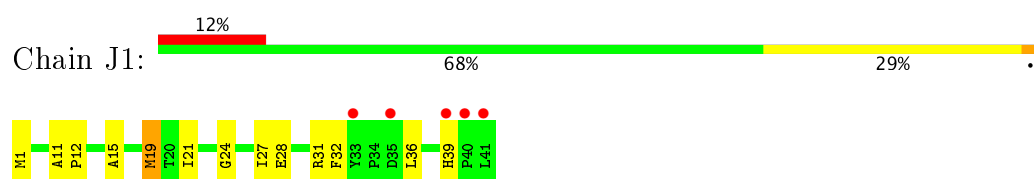


- Molecule 7: Photosystem I reaction center subunit VIII

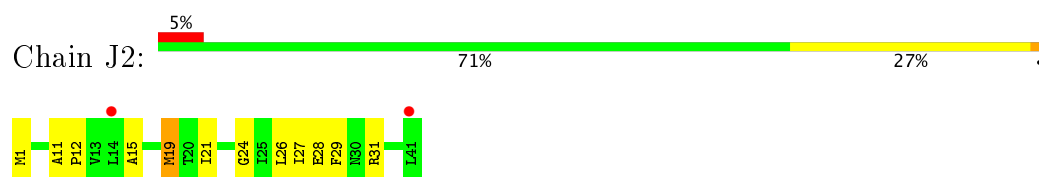


- Molecule 8: Photosystem I reaction center subunit IX

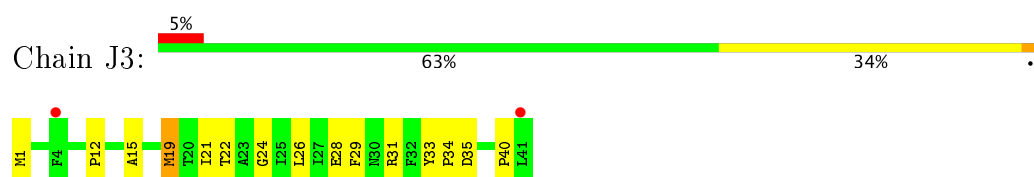




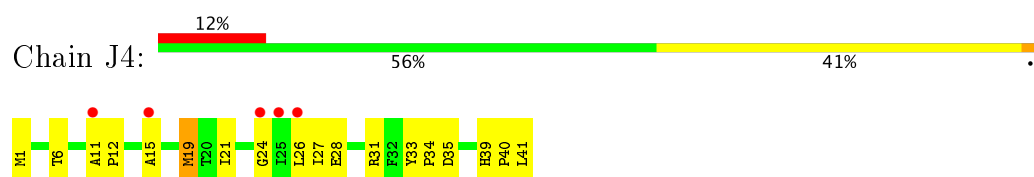
- Molecule 8: Photosystem I reaction center subunit IX



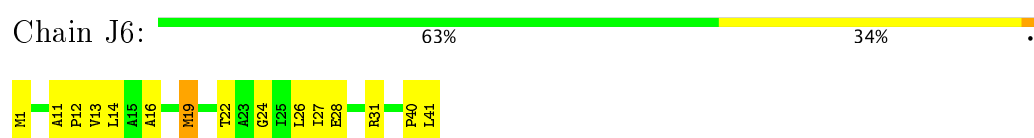
- Molecule 8: Photosystem I reaction center subunit IX



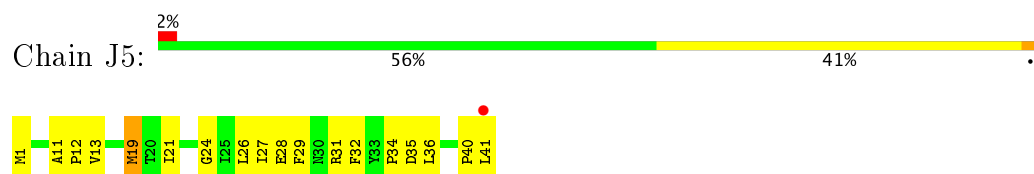
- Molecule 8: Photosystem I reaction center subunit IX



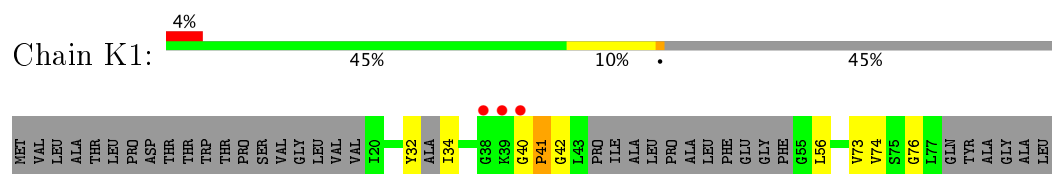
- Molecule 8: Photosystem I reaction center subunit IX



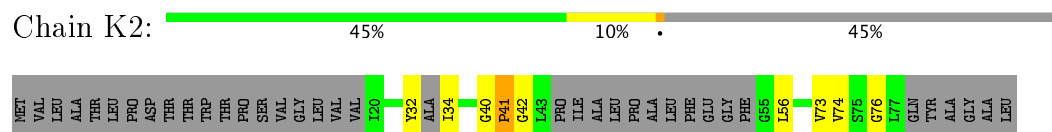
- Molecule 8: Photosystem I reaction center subunit IX



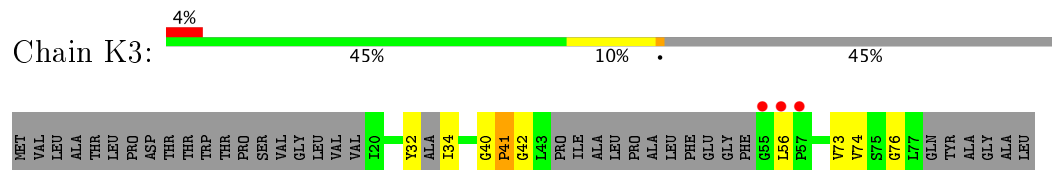
- Molecule 9: Photosystem I reaction center subunit Psak



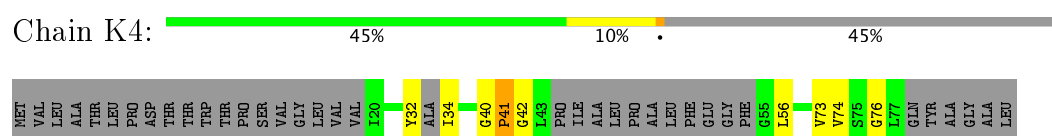
- Molecule 9: Photosystem I reaction center subunit Psak



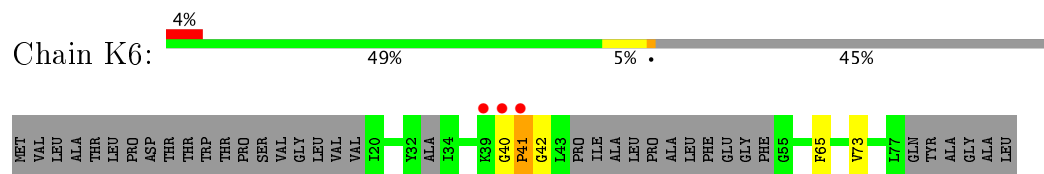
- Molecule 9: Photosystem I reaction center subunit PsaK



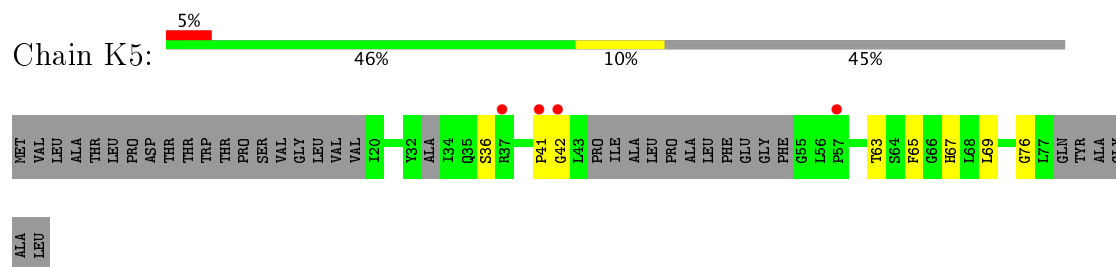
- Molecule 9: Photosystem I reaction center subunit PsaK



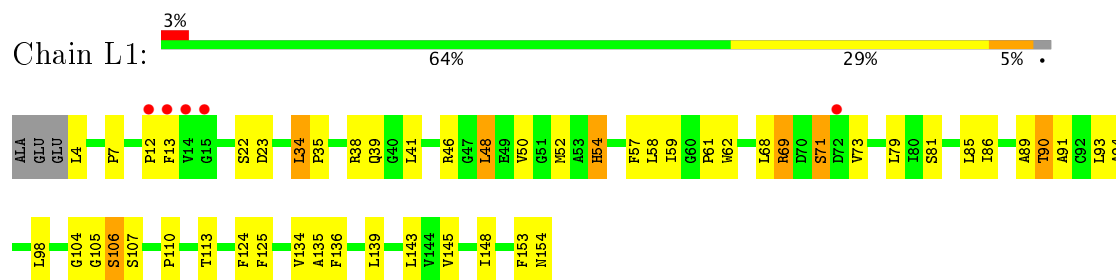
- Molecule 9: Photosystem I reaction center subunit PsaK



- Molecule 9: Photosystem I reaction center subunit PsaK

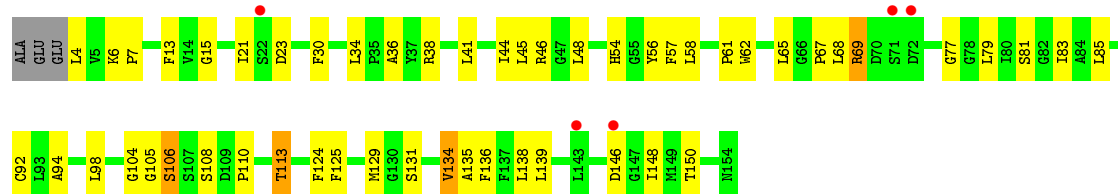


- Molecule 10: Photosystem I reaction center subunit XI

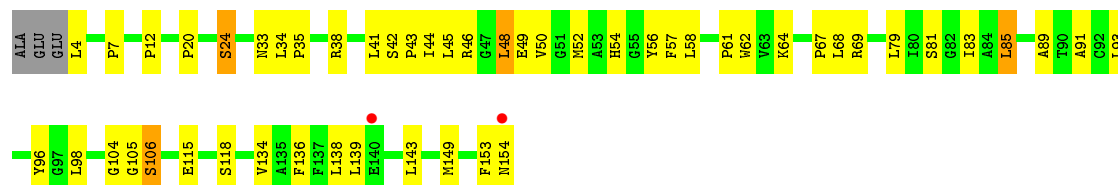


- Molecule 10: Photosystem I reaction center subunit XI

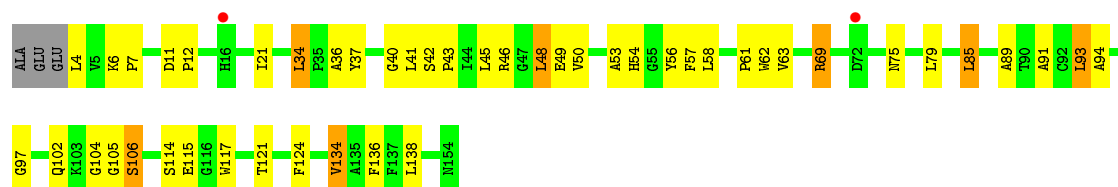




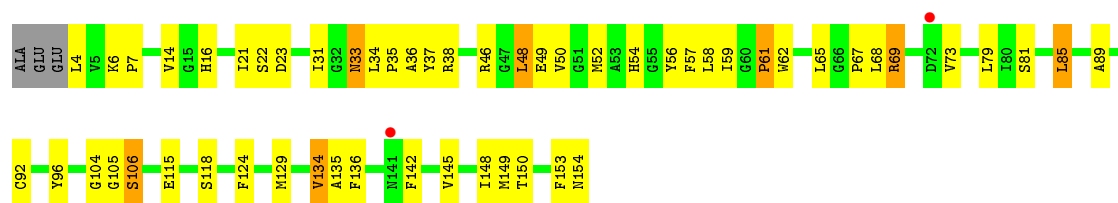
• Molecule 10: Photosystem I reaction center subunit XI



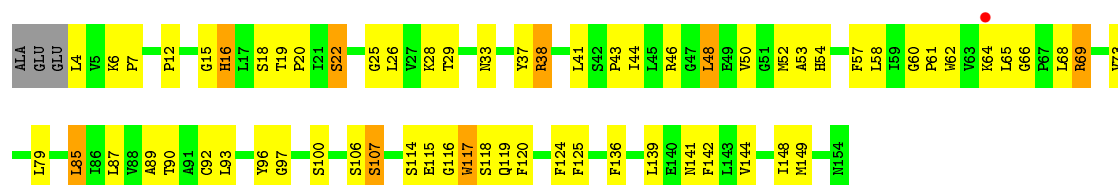
• Molecule 10: Photosystem I reaction center subunit XI



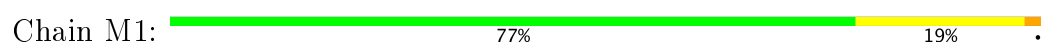
• Molecule 10: Photosystem I reaction center subunit XI



• 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



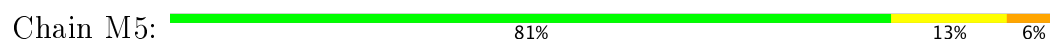
- Molecule 11: Photosystem I reaction center subunit XII



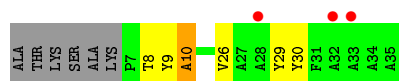
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Psax

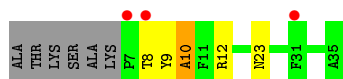


- Molecule 12: Psax

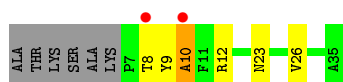




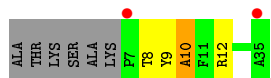
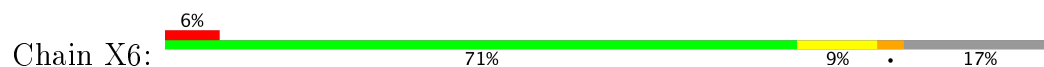
- Molecule 12: PsaX



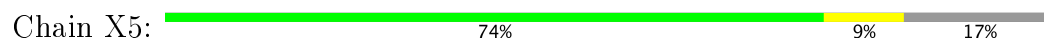
- Molecule 12: PsaX



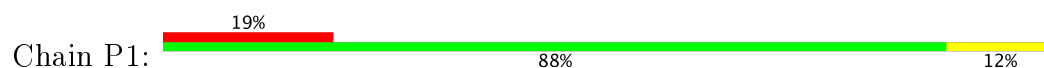
- Molecule 12: PsaX



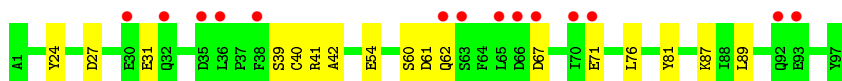
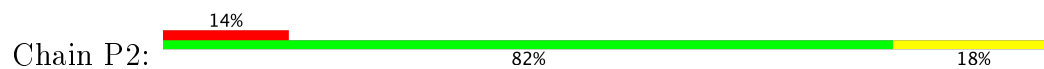
- Molecule 12: PsaX



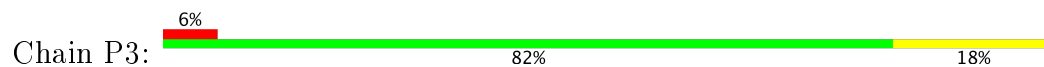
- Molecule 13: Ferredoxin-1

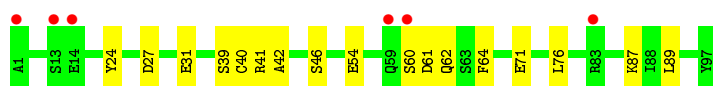


- Molecule 13: Ferredoxin-1

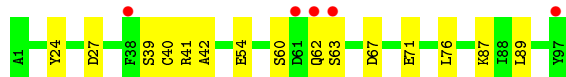
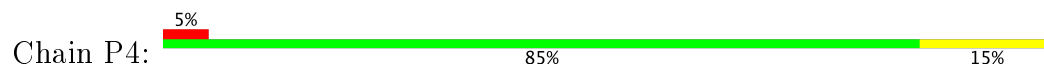


- Molecule 13: Ferredoxin-1

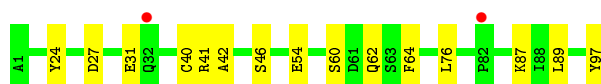
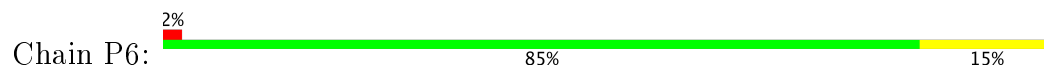




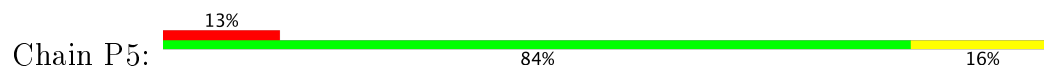
- Molecule 13: Ferredoxin-1



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	131.8	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 73.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

The worst 5 of 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

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 [i](#)

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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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
1	A2	736/755 (98%)	695 (94%)	33 (4%)	8 (1%)	16	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
6	F3	139/164 (85%)	127 (91%)	9 (6%)	3 (2%)	7	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
11	M4	29/31 (94%)	28 (97%)	0	1 (3%)	4	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

### 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
1	A2	589/603 (98%)	570 (97%)	19 (3%)	42	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
6	F3	109/128 (85%)	106 (97%)	3 (3%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
12	X4	20/24 (83%)	19 (95%)	1 (5%)	27	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 494 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E3	18	ASN
2	B4	146	SER
2	B5	453	GLU
7	I3	10	LEU
1	A4	147	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 170 such sidechains are listed below:

Mol	Chain	Res	Type
2	B3	688	HIS
2	B4	78	GLN
4	D5	54	ASN
4	D3	127	GLN
1	A4	50	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

The worst 5 of 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

5 of 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

5 of 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

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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A1	844	BCR	2	0
16	A1	845	BCR	2	0
16	A1	846	BCR	3	0
16	A1	847	BCR	19	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A2	1636	CLA	4	0
14	A2	1637	CLA	2	0
14	A2	1638	CLA	2	0
14	A2	1639	CLA	5	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A3	826	CLA	4	0
14	A3	827	CLA	3	0
14	A3	828	CLA	11	0
14	A3	829	CLA	4	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A4	812	CLA	1	0
14	A4	813	CLA	5	0
14	A4	814	CLA	2	0
14	A4	815	CLA	2	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A5	801	CLA	12	0
14	A5	802	CLA	5	0
14	A5	803	CLA	1	0
14	A5	804	CLA	4	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A5	844	PQN	2	0
16	A5	845	BCR	4	0
16	A5	846	BCR	2	0
16	A5	847	BCR	1	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A6	1632	CLA	1	0
14	A6	1633	CLA	9	0
14	A6	1634	CLA	3	0
14	A6	1635	CLA	2	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B1	824	CLA	7	0
14	B1	825	CLA	18	0
14	B1	826	CLA	12	0
14	B1	827	CLA	8	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B2	813	CLA	5	0
14	B2	814	CLA	4	0
14	B2	815	CLA	7	0
14	B2	816	CLA	14	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B3	1806	CLA	5	0
14	B3	1807	CLA	12	0
14	B3	1808	CLA	7	0
14	B3	1809	CLA	8	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B3	1849	BCR	5	0
19	B3	1850	LMG	8	0
16	B3	1851	BCR	3	0
14	B4	801	CLA	5	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B4	841	CLA	5	0
14	B4	842	CLA	5	0
14	B4	843	CLA	2	0
15	B4	844	PQN	7	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B5	1833	CLA	2	0
14	B5	1834	CLA	3	0
14	B5	1835	CLA	9	0
14	B5	1836	CLA	2	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B6	825	CLA	8	0
14	B6	826	CLA	6	0
14	B6	827	CLA	5	0
14	B6	828	CLA	11	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	F2	204	CLA	9	0
16	F3	201	BCR	2	0
14	F3	202	CLA	3	0
16	F3	203	BCR	1	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	J5	104	BCR	13	0
16	J5	105	BCR	4	0
14	J6	1101	CLA	4	0
14	J6	1102	CLA	3	0
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	L5	205	CLA	8	0
14	L5	206	CLA	7	0
16	L5	207	BCR	5	0
16	L6	201	BCR	4	0
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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	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 <sup>2</sup> )	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 <sup>2</sup> )	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%)

The worst 5 of 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

## 6.2 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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 [i](#)

There are no such residues in this entry.