



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:22 PM GMT

PDB ID : 4FE1
Title : Improving the Accuracy of Macromolecular Structure Refinement at 7 Å Resolution
Authors : Fromme, R.; Adams, P.D.; Fromme, P.; Levitt, M.; Schroeder, G.F.; Brunger, A.T.
Deposited on : 2012-05-29
Resolution : 4.92 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

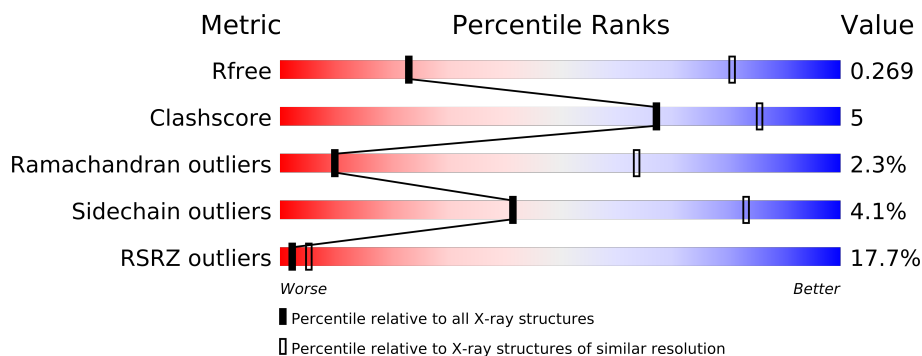
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 4.92 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1047 (6.22-3.50)
Clashscore	79885	1321 (6.22-3.50)
Ramachandran outliers	78287	1237 (6.22-3.50)
Sidechain outliers	78261	1217 (6.22-3.50)
RSRZ outliers	66119	1046 (6.22-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	755	
2	B	740	
3	C	80	
4	D	138	
5	E	75	
6	F	164	
7	I	38	
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
13	CLA	A	801	-	X
13	CLA	A	802	-	X
13	CLA	A	803	-	X
13	CLA	A	804	-	X
13	CLA	A	805	-	X
13	CLA	A	806	-	X
13	CLA	A	807	-	X
13	CLA	A	808	-	X
13	CLA	A	809	-	X
13	CLA	A	810	-	X
13	CLA	A	811	-	X
13	CLA	A	812	-	X
13	CLA	A	813	-	X
13	CLA	A	814	-	X
13	CLA	A	815	-	X
13	CLA	A	816	-	X
13	CLA	A	817	-	X
13	CLA	A	818	-	X
13	CLA	A	819	-	X
13	CLA	A	820	-	X
13	CLA	A	821	-	X
13	CLA	A	822	-	X
13	CLA	A	823	-	X
13	CLA	A	824	-	X
13	CLA	A	826	-	X
13	CLA	A	827	-	X
13	CLA	A	828	-	X
13	CLA	A	829	-	X
13	CLA	A	830	-	X
13	CLA	A	831	-	X
13	CLA	A	832	-	X
13	CLA	A	833	-	X
13	CLA	A	834	-	X
13	CLA	A	835	-	X
13	CLA	A	836	-	X
13	CLA	A	838	-	X
13	CLA	A	840	-	X
13	CLA	A	841	-	X
13	CLA	A	842	-	X
13	CLA	A	843	-	X
13	CLA	A	844	-	X
13	CLA	A	845	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
13	CLA	A	855	-	X
13	CLA	B	802	-	X
13	CLA	B	803	-	X
13	CLA	B	804	-	X
13	CLA	B	805	-	X
13	CLA	B	807	-	X
13	CLA	B	808	-	X
13	CLA	B	810	-	X
13	CLA	B	811	-	X
13	CLA	B	812	-	X
13	CLA	B	813	-	X
13	CLA	B	814	-	X
13	CLA	B	815	-	X
13	CLA	B	816	-	X
13	CLA	B	817	-	X
13	CLA	B	818	-	X
13	CLA	B	819	-	X
13	CLA	B	820	-	X
13	CLA	B	821	-	X
13	CLA	B	822	-	X
13	CLA	B	823	-	X
13	CLA	B	824	-	X
13	CLA	B	826	-	X
13	CLA	B	827	-	X
13	CLA	B	828	-	X
13	CLA	B	829	-	X
13	CLA	B	830	-	X
13	CLA	B	831	-	X
13	CLA	B	832	-	X
13	CLA	B	833	-	X
13	CLA	B	834	-	X
13	CLA	B	835	-	X
13	CLA	B	836	-	X
13	CLA	B	838	-	X
13	CLA	B	839	-	X
13	CLA	F	1301	-	X
13	CLA	J	1101	-	X
13	CLA	J	1102	-	X
13	CLA	J	1103	-	X
13	CLA	L	1003	-	X
13	CLA	L	1004	-	X
13	CLA	M	1201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
13	CLA	M	1202	-	X
13	CLA	X	102	-	X
14	PQN	A	846	-	X
14	PQN	B	840	-	X
15	BCR	A	847	-	X
15	BCR	A	848	-	X
15	BCR	A	849	-	X
15	BCR	A	850	-	X
15	BCR	A	851	-	X
15	BCR	A	852	-	X
15	BCR	B	841	-	X
15	BCR	B	842	-	X
15	BCR	B	843	-	X
15	BCR	B	844	-	X
15	BCR	B	845	-	X
15	BCR	B	846	-	X
15	BCR	B	847	-	X
15	BCR	B	849	-	X
15	BCR	B	850	-	X
15	BCR	F	1302	-	X
15	BCR	I	102	-	X
15	BCR	J	1104	-	X
15	BCR	J	1105	-	X
15	BCR	L	1005	-	X
15	BCR	M	1203	-	X
16	LHG	A	853	-	X
16	LHG	A	854	-	X
16	LHG	X	101	-	X
18	LMG	B	848	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 23997 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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	B	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	C	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	D	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	E	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	F	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	I	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	J	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	K	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	L	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	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	M	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			

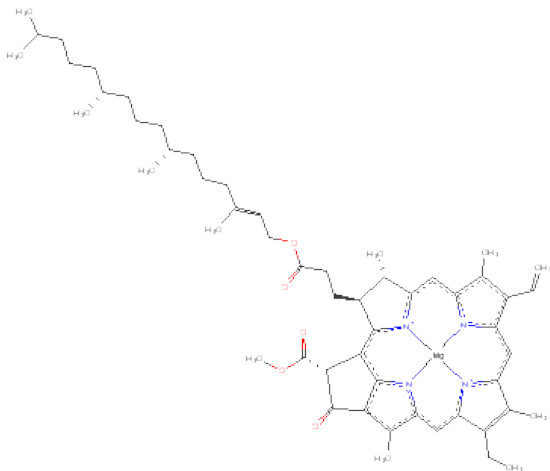
- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	29	Total	C	N	O	0	0	0
			233	164	34	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	32	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	33	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	34	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	35	ALA	-	EXPRESSION TAG	UNP Q8DKP6

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
13	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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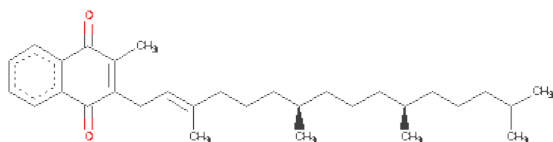
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	M	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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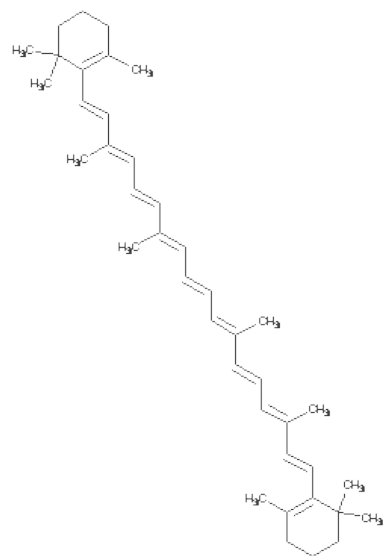
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			33	31	2		
14	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



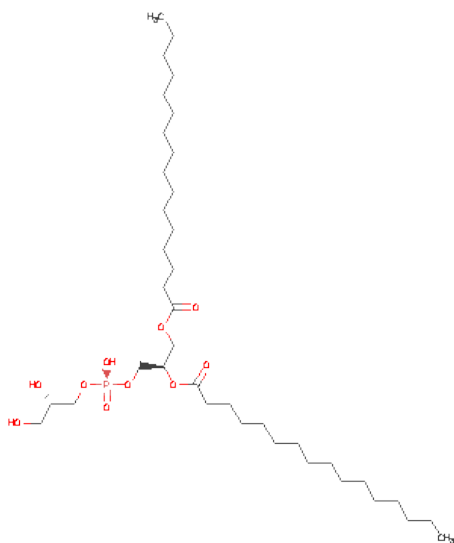
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 25 25	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0

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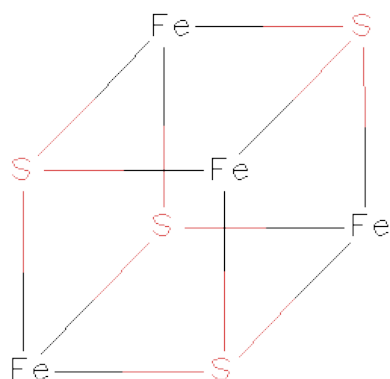
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C 40 40	0	0
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	M	1	Total C 40 40	0	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



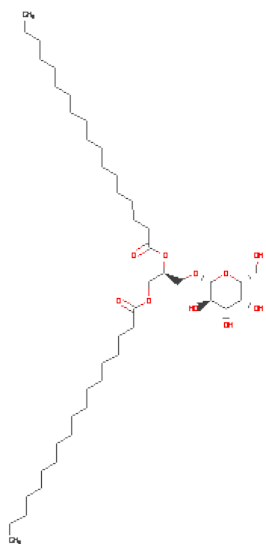
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 27 16 10 1	0	0
16	X	1	Total C O P 23 12 10 1	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	A	1	Total	Fe	S	0	0
			8	4	4		
17	C	1	Total	Fe	S	0	0
			8	4	4		
17	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	B	1	Total	C	O	0	0
			55	45	10		

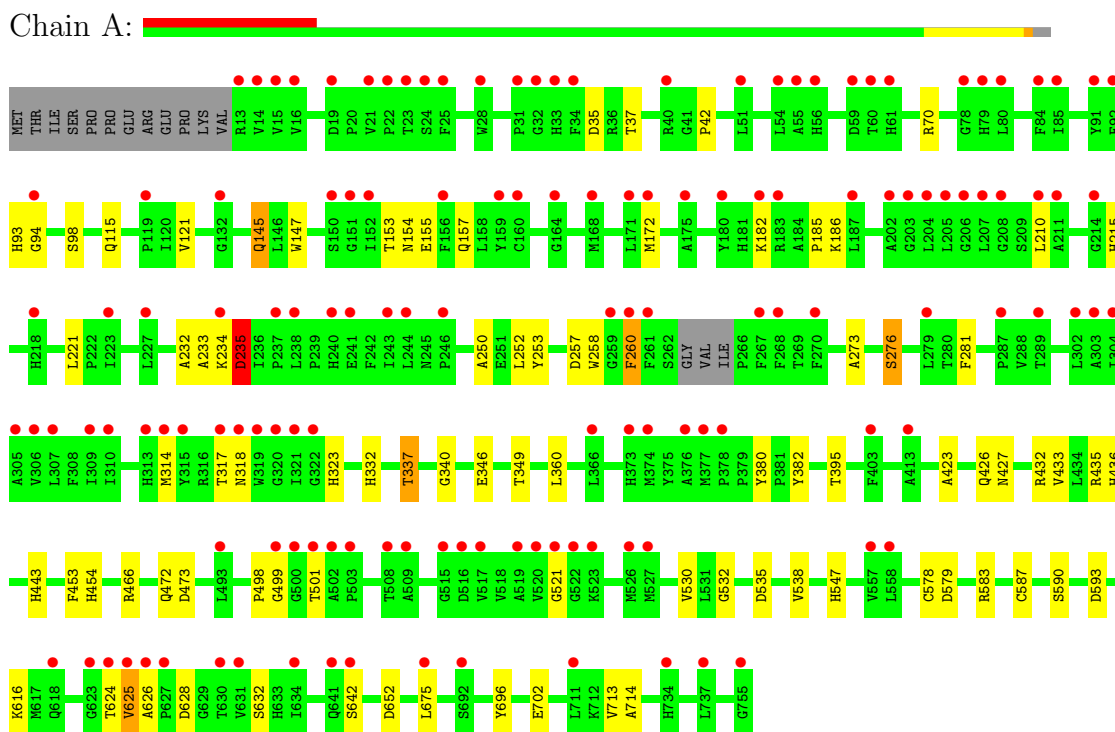
- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	1	Total	Ca	0	0
			1	1		

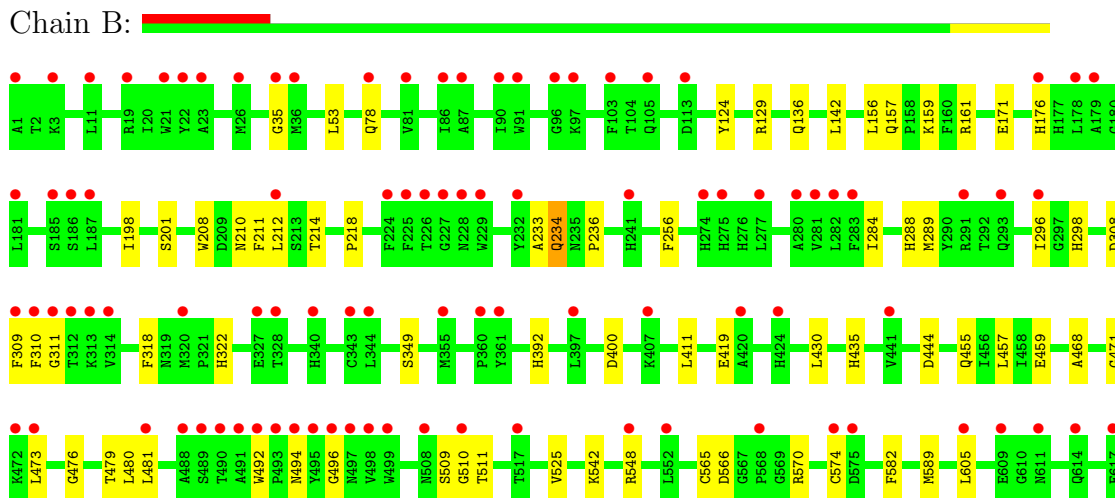
3 Residue-property plots

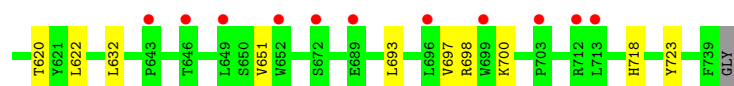
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



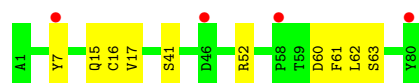
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





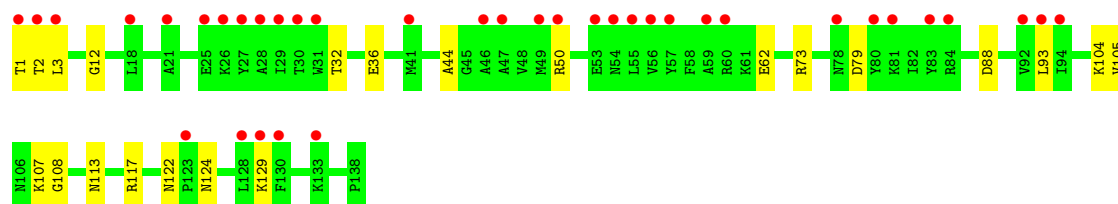
- Molecule 3: Photosystem I iron-sulfur center

Chain C:



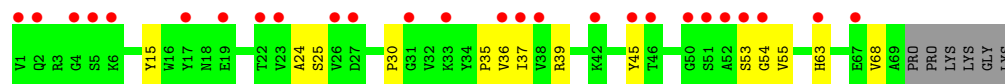
- Molecule 4: Photosystem I reaction center subunit II

Chain D:



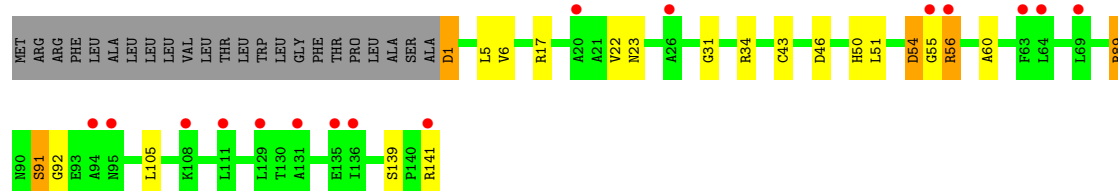
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:



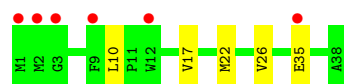
- Molecule 6: Photosystem I reaction center subunit III

Chain F:



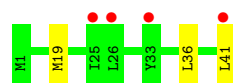
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



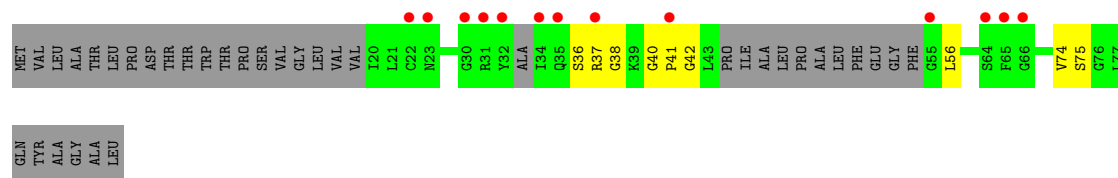
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:



- Molecule 9: Photosystem I reaction center subunit Psak

Chain K: 



- Molecule 10: Photosystem I reaction center subunit XI

Chain L: 



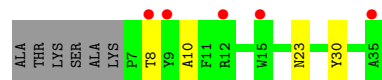
- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 



- Molecule 12: Photosystem I 4.8K protein

Chain X: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.97 – 4.92 97.97 – 4.92	Depositor EDS
% Data completeness (in resolution range)	96.4 (97.97-4.92) 96.3 (97.97-4.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.35 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1058)	Depositor
R, R_{free}	0.274 , 0.315 0.240 , 0.269	Depositor DCC
R_{free} test set	1526 reflections (4.69%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 90.2	EDS
Estimated twinning fraction	0.175 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Outliers	0 of 32897 reflections	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, SF4, CLA, PQN, 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	A	0.38	0/5983	0.69	3/8158 (0.0%)
2	B	0.40	0/6096	0.68	2/8332 (0.0%)
3	C	0.39	0/608	0.76	0/824
4	D	0.35	0/1101	0.78	0/1492
5	E	0.42	0/551	0.85	1/750 (0.1%)
6	F	0.41	0/1087	0.76	0/1476
7	I	0.38	0/312	0.80	1/425 (0.2%)
8	J	0.40	0/350	0.80	1/477 (0.2%)
9	K	0.40	0/220	0.91	0/300
10	L	0.39	0/1148	0.79	2/1558 (0.1%)
11	M	0.47	0/244	0.91	1/332 (0.3%)
12	X	0.41	0/242	0.66	0/332
All	All	0.39	0/17942	0.72	11/24456 (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
1	A	0	1
2	B	0	1
4	D	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD2	-8.44	110.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD1	8.11	125.60	118.30
10	L	76	LEU	CB-CG-CD2	7.19	123.22	111.00
7	I	26	VAL	CG1-CB-CG2	6.87	121.90	110.90
10	L	48	LEU	CB-CG-CD2	6.78	122.52	111.00
2	B	289	MET	CG-SD-CE	-5.94	90.70	100.20
11	M	17	LEU	CA-CB-CG	5.80	128.64	115.30
8	J	41	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	521	GLY	N-CA-C	-5.52	99.29	113.10
5	E	39	ARG	NE-CZ-NH1	-5.37	117.61	120.30
2	B	78	GLN	CA-CB-CG	5.04	124.48	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	THR	Mainchain
2	B	35	GLY	Mainchain
4	D	88	ASP	Mainchain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	0	46	0
2	B	5879	0	0	33	0
3	C	598	0	0	6	0
4	D	1075	0	0	8	0
5	E	539	0	0	3	0
6	F	1065	0	0	13	0
7	I	301	0	0	2	0
8	J	338	0	0	1	0
9	K	222	0	0	1	0
10	L	1119	0	0	7	1
11	M	241	0	0	2	0
12	X	233	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	2667	0	0	24	0
13	B	2230	0	0	14	0
13	F	45	0	0	1	0
13	I	65	0	0	1	0
13	J	147	0	0	0	0
13	L	195	0	0	1	0
13	M	99	0	0	1	0
13	X	45	0	0	0	0
14	A	33	0	0	0	0
14	B	33	0	0	0	0
15	A	240	0	0	0	0
15	B	345	0	0	0	0
15	F	40	0	0	0	0
15	I	40	0	0	0	0
15	J	80	0	0	0	0
15	L	80	0	0	1	0
15	M	40	0	0	0	0
16	A	76	0	0	0	0
16	X	23	0	0	0	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	B	55	0	0	0	0
19	L	1	0	0	0	0
All	All	23997	0	0	121	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (121) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:136:GLN:NE2	13:B:812:CLA:O1D	2.09	0.85
10:L:98:LEU:O	10:L:102:GLN:NE2	2.13	0.82
1:A:35:ASP:OD2	1:A:37:THR:OG1	2.02	0.78
1:A:501:THR:O	13:A:836:CLA:ND	2.20	0.74
6:F:91:SER:OG	6:F:92:GLY:N	2.24	0.70
2:B:509:SER:O	2:B:511:THR:N	2.27	0.67
9:K:36:SER:O	9:K:38:GLY:N	2.27	0.67
6:F:22:VAL:O	6:F:34:ARG:NH2	2.29	0.66
3:C:41:SER:OG	4:D:113:ASN:ND2	2.30	0.65
2:B:548:ARG:NH2	4:D:124:ASN:OD1	2.30	0.65
3:C:7:TYR:OH	4:D:122:ASN:ND2	2.30	0.64
1:A:70:ARG:NE	1:A:185:PRO:O	2.31	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:24:ALA:N	5:E:37:ILE:O	2.31	0.64
6:F:6:VAL:O	6:F:43:CYS:N	2.30	0.64
1:A:94:GLY:O	1:A:98:SER:OG	2.16	0.63
6:F:1:ASP:N	6:F:5:LEU:O	2.32	0.63
7:I:17:VAL:O	7:I:22:MET:N	2.33	0.62
6:F:54:ASP:O	6:F:56:ARG:N	2.33	0.62
1:A:153:THR:N	1:A:157:GLN:OE1	2.33	0.62
1:A:435:ARG:NH1	4:D:12:GLY:O	2.34	0.60
2:B:210:ASN:O	2:B:212:LEU:N	2.35	0.60
1:A:427:ASN:OD1	1:A:432:ARG:NH1	2.34	0.60
2:B:459:GLU:OE2	6:F:50:HIS:ND1	2.35	0.60
10:L:153:PHE:O	10:L:154:ASN:CB	2.50	0.59
2:B:693:LEU:N	10:L:37:TYR:OH	2.36	0.59
1:A:253:TYR:O	1:A:258:TRP:NE1	2.36	0.58
1:A:145:GLN:NE2	1:A:382:TYR:O	2.37	0.58
6:F:139:SER:O	6:F:141:ARG:NH1	2.37	0.58
2:B:419:GLU:OE1	6:F:141:ARG:NH2	2.37	0.57
2:B:455:GLN:OE1	2:B:620:THR:OG1	2.22	0.57
1:A:472:GLN:N	1:A:472:GLN:OE1	2.38	0.57
2:B:156:LEU:O	2:B:161:ARG:NH1	2.37	0.57
1:A:473:ASP:OD1	10:L:69:ARG:NH2	2.38	0.56
1:A:532:GLY:N	1:A:535:ASP:OD1	2.38	0.56
1:A:273:ALA:O	1:A:276:SER:OG	2.24	0.55
2:B:392:HIS:CE1	13:B:827:CLA:NA	2.76	0.53
1:A:714:ALA:O	6:F:89:ARG:NH2	2.42	0.53
3:C:7:TYR:N	3:C:63:SER:O	2.42	0.53
1:A:323:HIS:CE1	13:A:822:CLA:NA	2.77	0.53
2:B:284:ILE:O	2:B:288:HIS:ND1	2.42	0.52
2:B:400:ASP:OD1	4:D:129:LYS:NZ	2.43	0.52
1:A:93:HIS:CE1	13:A:807:CLA:NA	2.78	0.52
2:B:298:HIS:ND1	13:B:820:CLA:OBD	2.42	0.52
1:A:332:HIS:CE1	13:A:823:CLA:C1A	2.93	0.52
1:A:346:GLU:OE1	1:A:346:GLU:N	2.42	0.52
1:A:233:ALA:O	1:A:235:ASP:N	2.43	0.51
10:L:29:THR:O	10:L:33:ASN:ND2	2.44	0.51
1:A:215:HIS:CE1	13:A:814:CLA:C1A	2.92	0.51
2:B:124:TYR:O	2:B:129:ARG:NH1	2.44	0.51
1:A:436:HIS:CE1	13:A:831:CLA:C4D	2.93	0.51
1:A:590:SER:OG	1:A:593:ASP:OD2	2.29	0.50
1:A:696:TYR:O	2:B:542:LYS:NZ	2.44	0.50
13:B:806:CLA:CAA	13:B:806:CLA:CGD	2.89	0.50
1:A:215:HIS:CE1	13:A:814:CLA:NA	2.79	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:332:HIS:CE1	13:A:823:CLA:NA	2.81	0.48
2:B:473:LEU:O	2:B:476:GLY:N	2.46	0.48
1:A:530:VAL:O	1:A:616:LYS:NZ	2.45	0.48
2:B:700:LYS:NZ	7:I:35:GLU:O	2.47	0.48
1:A:154:ASN:N	1:A:157:GLN:OE1	2.46	0.48
3:C:60:ASP:OD2	5:E:15:TYR:N	2.47	0.48
6:F:17:ARG:NH2	6:F:46:ASP:O	2.46	0.48
2:B:509:SER:O	2:B:509:SER:OG	2.32	0.47
13:A:843:CLA:CGD	13:A:843:CLA:CAA	2.93	0.47
1:A:702:GLU:OE2	5:E:45:TYR:OH	2.33	0.47
13:B:831:CLA:CED	8:J:36:LEU:N	2.78	0.47
13:A:824:CLA:CAA	13:A:824:CLA:CGD	2.93	0.47
13:A:818:CLA:CAA	13:A:818:CLA:O1D	2.62	0.46
13:A:814:CLA:CGD	13:A:814:CLA:CAA	2.93	0.46
1:A:579:ASP:OD1	3:C:52:ARG:NH2	2.48	0.46
2:B:566:ASP:OD2	2:B:570:ARG:NH2	2.48	0.46
2:B:435:HIS:CE1	13:B:830:CLA:C4D	2.99	0.46
1:A:642:SER:OG	1:A:652:ASP:OD1	2.33	0.46
1:A:380:TYR:OH	13:A:829:CLA:O1D	2.34	0.46
1:A:454:HIS:CE1	13:A:833:CLA:C4D	2.98	0.46
1:A:547:HIS:CE1	13:A:839:CLA:C1A	2.99	0.46
2:B:309:PHE:O	2:B:311:GLY:N	2.49	0.45
13:A:817:CLA:CGD	13:A:817:CLA:CAA	2.94	0.45
13:A:829:CLA:CAA	13:A:829:CLA:CGD	2.94	0.45
1:A:436:HIS:CD2	13:A:831:CLA:NA	2.85	0.45
13:F:1301:CLA:CAA	13:F:1301:CLA:O1D	2.65	0.45
2:B:176:HIS:CE1	13:B:810:CLA:NA	2.84	0.45
13:L:1002:CLA:CAA	13:L:1002:CLA:CGD	2.95	0.45
6:F:54:ASP:OD1	12:X:30:TYR:CE2	2.69	0.45
2:B:208:TRP:NE1	13:B:812:CLA:O1D	2.50	0.45
13:B:820:CLA:CGD	13:B:820:CLA:CAA	2.95	0.44
1:A:337:THR:O	1:A:340:GLY:N	2.50	0.44
13:A:837:CLA:O2D	13:A:837:CLA:CAA	2.65	0.44
1:A:260:PHE:CD1	1:A:260:PHE:N	2.84	0.44
2:B:718:HIS:CE1	13:B:839:CLA:C4D	3.00	0.44
1:A:317:THR:OG1	1:A:318:ASN:N	2.49	0.43
6:F:23:ASN:OD1	6:F:31:GLY:N	2.51	0.43
2:B:198:ILE:O	2:B:201:SER:OG	2.36	0.43
2:B:308:ASP:O	13:B:820:CLA:CBA	2.66	0.43
2:B:157:GLN:NE2	11:M:28:GLU:OE1	2.51	0.43
13:B:829:CLA:CAA	13:B:829:CLA:CGD	2.96	0.43
1:A:547:HIS:CE1	13:A:839:CLA:NA	2.87	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:L:34:LEU:O	10:L:38:ARG:N	2.52	0.43
4:D:32:THR:OG1	4:D:79:ASP:OD2	2.36	0.43
1:A:453:PHE:O	13:A:834:CLA:CBB	2.67	0.43
2:B:233:ALA:O	2:B:234:GLN:O	2.37	0.42
1:A:443:HIS:CE1	13:A:832:CLA:NA	2.86	0.42
15:L:1006:BCR:C33	15:L:1006:BCR:C8	2.97	0.42
13:A:842:CLA:CAA	13:A:842:CLA:CGD	2.98	0.42
2:B:468:ALA:O	2:B:471:GLY:N	2.53	0.42
1:A:624:THR:OG1	1:A:625:VAL:N	2.52	0.42
3:C:16:CYS:SG	3:C:17:VAL:N	2.93	0.42
10:L:137:PHE:O	10:L:141:ASN:ND2	2.52	0.42
2:B:444:ASP:OD2	2:B:622:LEU:N	2.53	0.42
1:A:215:HIS:CD2	1:A:215:HIS:C	2.93	0.41
2:B:494:ASN:OD1	2:B:496:GLY:N	2.53	0.41
1:A:626:ALA:C	1:A:628:ASP:N	2.73	0.41
2:B:457:LEU:O	6:F:51:LEU:N	2.53	0.41
11:M:26:SER:O	13:M:1201:CLA:CGA	2.68	0.41
1:A:583:ARG:NH2	4:D:62:GLU:OE1	2.54	0.41
13:B:821:CLA:CAA	13:B:821:CLA:CGD	2.97	0.41
13:A:838:CLA:CAA	13:A:838:CLA:CGD	2.98	0.41
2:B:723:TYR:CE1	13:B:801:CLA:CGA	3.04	0.41
13:I:101:CLA:CGD	13:I:101:CLA:CAA	2.99	0.41
1:A:314:MET:O	1:A:323:HIS:N	2.54	0.41
4:D:36:GLU:OE2	4:D:50:ARG:NH2	2.55	0.40
1:A:423:ALA:O	1:A:426:GLN:NE2	2.54	0.40

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:L:40:GLY:O	10:L:114:SER:OG[3_665]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/755 (98%)	685 (93%)	39 (5%)	12 (2%)	14	71
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	19	77
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	18	75
4	D	136/138 (99%)	123 (90%)	8 (6%)	5 (4%)	5	52
5	E	67/75 (89%)	53 (79%)	6 (9%)	8 (12%)	1	14
6	F	139/164 (85%)	127 (91%)	8 (6%)	4 (3%)	7	58
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	42/83 (51%)	30 (71%)	5 (12%)	7 (17%)	0	7
10	L	149/154 (97%)	138 (93%)	9 (6%)	2 (1%)	18	75
11	M	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	6	55
12	X	27/35 (77%)	21 (78%)	5 (18%)	1 (4%)	5	52
All	All	2215/2334 (95%)	2039 (92%)	126 (6%)	50 (2%)	10	63

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	235	ASP
2	B	211	PHE
2	B	234	GLN
2	B	480	LEU
2	B	492	TRP
2	B	510	GLY
3	C	62	LEU
4	D	2	THR
6	F	55	GLY
6	F	91	SER
9	K	37	ARG
9	K	41	PRO
9	K	42	GLY
12	X	10	ALA
1	A	578	CYS
2	B	236	PRO
2	B	565	CYS
4	D	3	LEU
5	E	36	VAL
5	E	55	VAL
6	F	60	ALA

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Mol	Chain	Res	Type
9	K	74	VAL
10	L	104	GLY
10	L	106	SER
1	A	115	GLN
1	A	234	LYS
1	A	499	GLY
2	B	310	PHE
4	D	44	ALA
5	E	53	SER
6	F	89	ARG
9	K	75	SER
1	A	232	ALA
1	A	250	ALA
1	A	625	VAL
4	D	107	LYS
5	E	25	SER
5	E	35	PRO
5	E	68	VAL
1	A	42	PRO
1	A	182	LYS
1	A	498	PRO
2	B	481	LEU
4	D	108	GLY
11	M	30	TYR
5	E	30	PRO
9	K	40	GLY
9	K	56	LEU
5	E	54	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/603 (98%)	567 (96%)	22 (4%)	45	85
2	B	595/597 (100%)	572 (96%)	23 (4%)	43	84
3	C	67/67 (100%)	65 (97%)	2 (3%)	53	88
4	D	115/115 (100%)	109 (95%)	6 (5%)	32	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	59/64 (92%)	58 (98%)	1 (2%)	73	94
6	F	109/128 (85%)	105 (96%)	4 (4%)	45	85
7	I	32/32 (100%)	31 (97%)	1 (3%)	52	88
8	J	36/36 (100%)	35 (97%)	1 (3%)	56	88
10	L	117/119 (98%)	109 (93%)	8 (7%)	22	69
11	M	26/26 (100%)	24 (92%)	2 (8%)	18	64
12	X	20/24 (83%)	18 (90%)	2 (10%)	11	51
All	All	1765/1811 (98%)	1693 (96%)	72 (4%)	41	83

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	147	TRP
1	A	155	GLU
1	A	172	MET
1	A	186	LYS
1	A	210	LEU
1	A	221	LEU
1	A	235	ASP
1	A	252	LEU
1	A	260	PHE
1	A	276	SER
1	A	281	PHE
1	A	349	THR
1	A	360	LEU
1	A	395	THR
1	A	433	VAL
1	A	466	ARG
1	A	538	VAL
1	A	587	CYS
1	A	632	SER
1	A	675	LEU
1	A	713	VAL
2	B	53	LEU
2	B	142	LEU
2	B	159	LYS
2	B	171	GLU
2	B	214	THR
2	B	218	PRO

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Mol	Chain	Res	Type
2	B	256	PHE
2	B	296	ILE
2	B	318	PHE
2	B	322	HIS
2	B	349	SER
2	B	411	LEU
2	B	430	LEU
2	B	479	THR
2	B	525	VAL
2	B	574	CYS
2	B	582	PHE
2	B	589	MET
2	B	605	LEU
2	B	632	LEU
2	B	651	VAL
2	B	697	VAL
2	B	698	ARG
3	C	15	GLN
3	C	61	PHE
4	D	1	THR
4	D	73	ARG
4	D	93	LEU
4	D	104	LYS
4	D	105	VAL
4	D	117	ARG
5	E	63	HIS
6	F	1	ASP
6	F	54	ASP
6	F	56	ARG
6	F	105	LEU
7	I	10	LEU
8	J	19	MET
10	L	4	LEU
10	L	34	LEU
10	L	44	ILE
10	L	48	LEU
10	L	69	ARG
10	L	85	LEU
10	L	134	VAL
10	L	142	PHE
11	M	3	LEU
11	M	17	LEU

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Mol	Chain	Res	Type
12	X	8	THR
12	X	23	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 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$
13	CLA	A	801	-	73,73,73	1.51	15 (20%)	95,113,113	1.95	20 (21%)
13	CLA	A	802	-	73,73,73	1.51	15 (20%)	95,113,113	1.46	13 (13%)
13	CLA	A	803	-	73,73,73	1.48	13 (17%)	95,113,113	1.64	16 (16%)
13	CLA	A	804	13	67,67,73	1.58	15 (22%)	86,105,113	1.69	16 (18%)
13	CLA	A	805	-	73,73,73	1.49	13 (17%)	95,113,113	1.58	14 (14%)
13	CLA	A	806	-	73,73,73	1.46	13 (17%)	95,113,113	1.54	16 (16%)
13	CLA	A	807	-	59,59,73	1.79	16 (27%)	77,96,113	1.84	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	808	1	73,73,73	1.52	14 (19%)	95,113,113	1.93	20 (21%)
13	CLA	A	809	1	73,73,73	1.50	14 (19%)	95,113,113	1.87	22 (23%)
13	CLA	A	810	-	51,53,73	1.76	13 (25%)	68,89,113	2.01	14 (20%)
13	CLA	A	811	13	73,73,73	1.49	15 (20%)	95,113,113	1.74	16 (16%)
13	CLA	A	812	-	62,62,73	1.58	14 (22%)	80,99,113	1.85	16 (20%)
13	CLA	A	813	-	67,68,73	1.55	13 (19%)	87,107,113	1.82	22 (25%)
13	CLA	A	814	-	51,53,73	1.75	12 (23%)	68,89,113	1.89	12 (17%)
13	CLA	A	815	-	51,53,73	1.77	11 (21%)	68,89,113	1.86	12 (17%)
13	CLA	A	816	-	56,57,73	1.64	14 (25%)	73,93,113	1.75	14 (19%)
13	CLA	A	817	-	62,62,73	1.62	15 (24%)	80,99,113	1.70	15 (18%)
13	CLA	A	818	-	62,62,73	1.60	15 (24%)	80,99,113	1.88	18 (22%)
13	CLA	A	819	-	73,73,73	1.46	16 (21%)	95,113,113	1.78	20 (21%)
13	CLA	A	820	-	69,69,73	1.66	16 (23%)	89,108,113	1.62	17 (19%)
13	CLA	A	821	-	73,73,73	1.49	15 (20%)	95,113,113	1.65	18 (18%)
13	CLA	A	822	-	56,57,73	1.67	14 (25%)	73,93,113	2.08	15 (20%)
13	CLA	A	823	-	59,59,73	1.80	15 (25%)	77,96,113	1.51	14 (18%)
13	CLA	A	824	-	67,67,73	1.56	14 (20%)	86,105,113	2.13	20 (23%)
13	CLA	A	825	-	73,73,73	1.49	16 (21%)	95,113,113	1.61	18 (18%)
13	CLA	A	826	-	73,73,73	1.52	14 (19%)	95,113,113	1.69	19 (20%)
13	CLA	A	827	-	73,73,73	1.47	14 (19%)	95,113,113	1.72	18 (18%)
13	CLA	A	828	-	73,73,73	1.49	15 (20%)	95,113,113	1.75	16 (16%)
13	CLA	A	829	-	73,73,73	1.47	14 (19%)	95,113,113	1.76	17 (17%)
13	CLA	A	830	-	73,73,73	1.46	15 (20%)	95,113,113	1.78	17 (17%)
13	CLA	A	831	-	58,58,73	1.66	14 (24%)	75,95,113	1.70	14 (18%)
13	CLA	A	832	-	73,73,73	1.48	14 (19%)	95,113,113	1.77	16 (16%)
13	CLA	A	833	-	73,73,73	1.49	15 (20%)	95,113,113	1.57	15 (15%)
13	CLA	A	834	-	73,73,73	1.49	14 (19%)	95,113,113	1.60	13 (13%)
13	CLA	A	835	-	62,62,73	1.62	14 (22%)	80,99,113	1.60	14 (17%)
13	CLA	A	836	1	51,53,73	1.76	11 (21%)	68,89,113	1.62	13 (19%)
13	CLA	A	837	-	59,59,73	1.85	15 (25%)	77,96,113	2.18	21 (27%)
13	CLA	A	838	-	73,73,73	1.50	14 (19%)	95,113,113	1.71	18 (18%)
13	CLA	A	839	-	54,55,73	1.61	12 (22%)	72,91,113	1.75	15 (20%)
13	CLA	A	840	-	73,73,73	1.48	16 (21%)	95,113,113	1.71	13 (13%)
13	CLA	A	841	-	59,59,73	1.80	15 (25%)	77,96,113	1.61	14 (18%)
13	CLA	A	842	-	73,73,73	1.52	16 (21%)	95,113,113	1.48	15 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	843	-	73,73,73	1.45	14 (19%)	95,113,113	1.71	20 (21%)
13	CLA	A	844	-	47,49,73	3.17	12 (25%)	59,83,113	1.64	8 (13%)
13	CLA	A	845	16	60,60,73	1.64	14 (23%)	79,97,113	1.91	20 (25%)
14	PQN	A	846	-	34,34,34	1.01	1 (2%)	45,45,45	1.11	3 (6%)
15	BCR	A	847	-	41,41,41	2.20	22 (53%)	56,56,56	2.04	22 (39%)
15	BCR	A	848	-	41,41,41	2.20	20 (48%)	56,56,56	2.13	20 (35%)
15	BCR	A	849	-	41,41,41	2.06	17 (41%)	56,56,56	2.21	25 (44%)
15	BCR	A	850	-	41,41,41	2.25	21 (51%)	56,56,56	2.18	20 (35%)
15	BCR	A	851	-	41,41,41	2.17	21 (51%)	56,56,56	2.16	19 (33%)
15	BCR	A	852	-	41,41,41	2.22	20 (48%)	56,56,56	2.25	18 (32%)
16	LHG	A	853	-	48,48,48	0.87	2 (4%)	54,54,54	1.01	2 (3%)
16	LHG	A	854	13	26,26,48	4.10	4 (15%)	31,32,54	1.59	3 (9%)
13	CLA	A	855	-	51,53,73	1.77	12 (23%)	68,89,113	1.83	14 (20%)
17	SF4	A	856	1,2	12,12,12	21.02	12 (100%)	0,24,24	0.00	-
13	CLA	B	801	-	73,73,73	1.50	13 (17%)	95,113,113	1.79	20 (21%)
13	CLA	B	802	-	73,73,73	1.51	15 (20%)	95,113,113	2.04	19 (20%)
13	CLA	B	803	-	73,73,73	1.50	15 (20%)	95,113,113	1.78	19 (20%)
13	CLA	B	804	-	73,73,73	1.47	15 (20%)	95,113,113	1.61	16 (16%)
13	CLA	B	805	-	73,73,73	1.47	14 (19%)	95,113,113	1.51	17 (17%)
13	CLA	B	806	-	73,73,73	1.48	15 (20%)	95,113,113	1.65	17 (17%)
13	CLA	B	807	-	73,73,73	1.50	16 (21%)	95,113,113	1.70	15 (15%)
13	CLA	B	808	2	73,73,73	1.49	15 (20%)	95,113,113	1.79	19 (20%)
13	CLA	B	809	-	51,53,73	1.74	12 (23%)	68,89,113	1.99	13 (19%)
13	CLA	B	810	-	51,53,73	1.85	11 (21%)	68,89,113	1.61	12 (17%)
13	CLA	B	811	-	73,73,73	1.52	14 (19%)	95,113,113	1.79	20 (21%)
13	CLA	B	812	-	73,73,73	1.49	15 (20%)	95,113,113	1.80	17 (17%)
13	CLA	B	813	-	51,53,73	1.79	11 (21%)	68,89,113	2.00	14 (20%)
13	CLA	B	814	-	62,63,73	1.59	15 (24%)	81,101,113	1.88	18 (22%)
13	CLA	B	815	-	67,67,73	1.57	14 (20%)	86,105,113	1.60	17 (19%)
13	CLA	B	816	-	67,68,73	1.57	12 (17%)	87,107,113	1.73	16 (18%)
13	CLA	B	817	-	73,73,73	1.48	17 (23%)	95,113,113	1.55	13 (13%)
13	CLA	B	818	-	54,55,73	1.64	12 (22%)	72,91,113	1.79	15 (20%)
13	CLA	B	819	-	51,53,73	1.81	12 (23%)	68,89,113	2.00	15 (22%)
13	CLA	B	820	-	62,63,73	1.62	16 (25%)	81,101,113	1.63	17 (20%)
13	CLA	B	821	-	51,53,73	1.83	13 (25%)	68,89,113	1.78	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	822	-	62,62,73	1.64	16 (25%)	80,99,113	1.84	19 (23%)
13	CLA	B	823	-	53,54,73	1.62	13 (24%)	71,90,113	1.84	18 (25%)
13	CLA	B	824	-	73,73,73	1.49	14 (19%)	95,113,113	1.81	19 (20%)
13	CLA	B	825	-	73,73,73	1.52	15 (20%)	95,113,113	1.57	15 (15%)
13	CLA	B	826	-	73,73,73	1.48	13 (17%)	95,113,113	1.42	11 (11%)
13	CLA	B	827	-	73,73,73	1.48	14 (19%)	95,113,113	1.90	19 (20%)
13	CLA	B	828	-	51,53,73	1.80	12 (23%)	68,89,113	1.91	14 (20%)
13	CLA	B	829	-	56,57,73	1.64	15 (26%)	73,93,113	1.67	12 (16%)
13	CLA	B	830	-	73,73,73	1.51	14 (19%)	95,113,113	1.59	13 (13%)
13	CLA	B	831	-	65,66,73	1.56	14 (21%)	85,104,113	2.14	19 (22%)
13	CLA	B	832	-	51,53,73	1.77	13 (25%)	68,89,113	1.88	13 (19%)
13	CLA	B	833	-	51,53,73	1.77	13 (25%)	68,89,113	1.81	14 (20%)
13	CLA	B	834	-	51,53,73	1.80	13 (25%)	68,89,113	1.88	14 (20%)
13	CLA	B	835	-	67,68,73	1.57	12 (17%)	87,107,113	1.93	20 (22%)
13	CLA	B	836	-	73,73,73	1.50	15 (20%)	95,113,113	1.60	16 (16%)
13	CLA	B	837	-	54,55,73	1.63	14 (25%)	72,91,113	1.82	15 (20%)
13	CLA	B	838	-	73,73,73	1.48	14 (19%)	95,113,113	1.74	20 (21%)
13	CLA	B	839	-	73,73,73	1.47	13 (17%)	95,113,113	1.58	16 (16%)
14	PQN	B	840	-	34,34,34	0.94	1 (2%)	45,45,45	1.28	4 (8%)
15	BCR	B	841	-	41,41,41	2.17	22 (53%)	56,56,56	2.09	21 (37%)
15	BCR	B	842	-	41,41,41	2.22	21 (51%)	56,56,56	2.27	20 (35%)
15	BCR	B	843	-	41,41,41	2.14	20 (48%)	56,56,56	2.39	25 (44%)
15	BCR	B	844	-	24,25,41	2.48	13 (54%)	31,33,56	2.29	13 (41%)
15	BCR	B	845	-	41,41,41	2.14	20 (48%)	56,56,56	2.34	21 (37%)
15	BCR	B	846	-	41,41,41	2.18	21 (51%)	56,56,56	2.06	21 (37%)
15	BCR	B	847	-	41,41,41	2.17	21 (51%)	56,56,56	2.27	23 (41%)
18	LMG	B	848	-	55,55,55	1.02	6 (10%)	63,63,63	1.18	3 (4%)
15	BCR	B	849	-	41,41,41	2.09	18 (43%)	56,56,56	2.33	22 (39%)
15	BCR	B	850	-	41,41,41	2.18	20 (48%)	56,56,56	2.36	23 (41%)
17	SF4	C	101	3	12,12,12	20.95	12 (100%)	0,24,24	0.00	-
17	SF4	C	102	3	12,12,12	20.83	12 (100%)	0,24,24	0.00	-
13	CLA	F	1301	-	51,53,73	1.89	12 (23%)	68,89,113	1.92	17 (25%)
15	BCR	F	1302	-	41,41,41	2.15	20 (48%)	56,56,56	2.19	21 (37%)
13	CLA	I	101	-	73,73,73	1.49	15 (20%)	95,113,113	1.72	16 (16%)
15	BCR	I	102	-	41,41,41	2.06	17 (41%)	56,56,56	2.32	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	J	1101	-	73,73,73	1.47	14 (19%)	95,113,113	1.70	22 (23%)
13	CLA	J	1102	8	51,53,73	1.79	12 (23%)	68,89,113	2.02	14 (20%)
13	CLA	J	1103	-	44,45,73	3.14	13 (29%)	55,78,113	1.61	7 (12%)
15	BCR	J	1104	-	41,41,41	2.20	21 (51%)	56,56,56	2.23	23 (41%)
15	BCR	J	1105	-	41,41,41	2.19	21 (51%)	56,56,56	2.13	22 (39%)
13	CLA	L	1002	10	73,73,73	1.49	14 (19%)	95,113,113	1.77	16 (16%)
13	CLA	L	1003	-	73,73,73	1.47	12 (16%)	95,113,113	1.85	17 (17%)
13	CLA	L	1004	-	73,73,73	1.47	13 (17%)	95,113,113	1.66	17 (17%)
15	BCR	L	1005	-	41,41,41	2.14	22 (53%)	56,56,56	2.24	22 (39%)
15	BCR	L	1006	-	41,41,41	2.19	20 (48%)	56,56,56	2.01	19 (33%)
13	CLA	M	1201	-	62,62,73	1.64	17 (27%)	80,99,113	1.88	19 (23%)
13	CLA	M	1202	-	51,53,73	1.84	13 (25%)	68,89,113	1.97	15 (22%)
15	BCR	M	1203	-	41,41,41	2.13	19 (46%)	56,56,56	2.27	19 (33%)
16	LHG	X	101	-	21,22,48	3.37	3 (14%)	26,28,54	1.04	2 (7%)
13	CLA	X	102	12	51,53,73	1.82	12 (23%)	68,89,113	2.20	14 (20%)

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
13	CLA	A	801	-	-	0/37/135/135	0/0/9/9
13	CLA	A	802	-	-	0/37/135/135	0/0/9/9
13	CLA	A	803	-	-	0/37/135/135	0/0/9/9
13	CLA	A	804	13	-	0/29/128/135	0/0/9/9
13	CLA	A	805	-	-	0/37/135/135	0/0/9/9
13	CLA	A	806	-	-	0/37/135/135	0/0/9/9
13	CLA	A	807	-	-	0/21/119/135	0/0/9/9
13	CLA	A	808	1	-	0/37/135/135	0/0/9/9
13	CLA	A	809	1	-	0/37/135/135	0/0/9/9
13	CLA	A	810	-	-	0/11/111/135	0/0/9/9
13	CLA	A	811	13	-	0/37/135/135	0/0/9/9
13	CLA	A	812	-	-	0/23/122/135	0/0/9/9
13	CLA	A	813	-	-	0/31/129/135	0/0/9/9
13	CLA	A	814	-	-	0/11/111/135	0/0/9/9
13	CLA	A	815	-	-	0/11/111/135	0/0/9/9
13	CLA	A	816	-	-	0/17/116/135	0/0/9/9
13	CLA	A	817	-	-	0/23/122/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	818	-	-	0/23/122/135	0/0/9/9
13	CLA	A	819	-	-	0/37/135/135	0/0/9/9
13	CLA	A	820	-	-	0/33/131/135	0/0/9/9
13	CLA	A	821	-	-	0/37/135/135	0/0/9/9
13	CLA	A	822	-	-	0/17/116/135	0/0/9/9
13	CLA	A	823	-	-	0/21/119/135	0/0/9/9
13	CLA	A	824	-	-	0/29/128/135	0/0/9/9
13	CLA	A	825	-	-	0/37/135/135	0/0/9/9
13	CLA	A	826	-	-	0/37/135/135	0/0/9/9
13	CLA	A	827	-	-	0/37/135/135	0/0/9/9
13	CLA	A	828	-	-	0/37/135/135	0/0/9/9
13	CLA	A	829	-	-	0/37/135/135	0/0/9/9
13	CLA	A	830	-	-	0/37/135/135	0/0/9/9
13	CLA	A	831	-	-	0/19/117/135	0/0/9/9
13	CLA	A	832	-	-	0/37/135/135	0/0/9/9
13	CLA	A	833	-	-	0/37/135/135	0/0/9/9
13	CLA	A	834	-	-	0/37/135/135	0/0/9/9
13	CLA	A	835	-	-	0/23/122/135	0/0/9/9
13	CLA	A	836	1	-	0/11/111/135	0/0/9/9
13	CLA	A	837	-	-	0/21/119/135	0/0/9/9
13	CLA	A	838	-	-	0/37/135/135	0/0/9/9
13	CLA	A	839	-	-	0/16/114/135	0/0/9/9
13	CLA	A	840	-	-	0/37/135/135	0/0/9/9
13	CLA	A	841	-	-	0/21/119/135	0/0/9/9
13	CLA	A	842	-	-	0/37/135/135	0/0/9/9
13	CLA	A	843	-	-	0/37/135/135	0/0/9/9
13	CLA	A	844	-	-	0/5/101/135	0/0/9/9
13	CLA	A	845	16	-	0/22/120/135	0/0/9/9
14	PQN	A	846	-	-	0/23/43/43	0/0/2/2
15	BCR	A	847	-	-	0/29/63/63	0/2/2/2
15	BCR	A	848	-	-	0/29/63/63	0/2/2/2
15	BCR	A	849	-	-	0/29/63/63	0/2/2/2
15	BCR	A	850	-	-	0/29/63/63	0/2/2/2
15	BCR	A	851	-	-	0/29/63/63	0/2/2/2
15	BCR	A	852	-	-	0/29/63/63	0/2/2/2
16	LHG	A	853	-	-	0/53/53/53	0/0/0/0
16	LHG	A	854	13	-	0/31/31/53	0/0/0/0
13	CLA	A	855	-	-	0/11/111/135	0/0/9/9
17	SF4	A	856	1,2	-	0/0/48/48	0/0/5/5
13	CLA	B	801	-	-	0/37/135/135	0/0/9/9
13	CLA	B	802	-	-	0/37/135/135	0/0/9/9
13	CLA	B	803	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	804	-	-	0/37/135/135	0/0/9/9
13	CLA	B	805	-	-	0/37/135/135	0/0/9/9
13	CLA	B	806	-	-	0/37/135/135	0/0/9/9
13	CLA	B	807	-	-	0/37/135/135	0/0/9/9
13	CLA	B	808	2	-	0/37/135/135	0/0/9/9
13	CLA	B	809	-	-	0/11/111/135	0/0/9/9
13	CLA	B	810	-	-	0/11/111/135	0/0/9/9
13	CLA	B	811	-	-	0/37/135/135	0/0/9/9
13	CLA	B	812	-	-	0/37/135/135	0/0/9/9
13	CLA	B	813	-	-	0/11/111/135	0/0/9/9
13	CLA	B	814	-	-	0/25/123/135	0/0/9/9
13	CLA	B	815	-	-	0/29/128/135	0/0/9/9
13	CLA	B	816	-	-	0/31/129/135	0/0/9/9
13	CLA	B	817	-	-	0/37/135/135	0/0/9/9
13	CLA	B	818	-	-	0/16/114/135	0/0/9/9
13	CLA	B	819	-	-	0/11/111/135	0/0/9/9
13	CLA	B	820	-	-	0/25/123/135	0/0/9/9
13	CLA	B	821	-	-	0/11/111/135	0/0/9/9
13	CLA	B	822	-	-	0/23/122/135	0/0/9/9
13	CLA	B	823	-	-	0/15/113/135	0/0/9/9
13	CLA	B	824	-	-	0/37/135/135	0/0/9/9
13	CLA	B	825	-	-	0/37/135/135	0/0/9/9
13	CLA	B	826	-	-	0/37/135/135	0/0/9/9
13	CLA	B	827	-	-	0/37/135/135	0/0/9/9
13	CLA	B	828	-	-	0/11/111/135	0/0/9/9
13	CLA	B	829	-	-	0/17/116/135	0/0/9/9
13	CLA	B	830	-	-	0/37/135/135	0/0/9/9
13	CLA	B	831	-	-	0/29/127/135	0/0/9/9
13	CLA	B	832	-	-	0/11/111/135	0/0/9/9
13	CLA	B	833	-	-	0/11/111/135	0/0/9/9
13	CLA	B	834	-	-	0/11/111/135	0/0/9/9
13	CLA	B	835	-	-	0/31/129/135	0/0/9/9
13	CLA	B	836	-	-	0/37/135/135	0/0/9/9
13	CLA	B	837	-	-	0/16/114/135	0/0/9/9
13	CLA	B	838	-	-	0/37/135/135	0/0/9/9
13	CLA	B	839	-	-	0/37/135/135	0/0/9/9
14	PQN	B	840	-	-	0/23/43/43	0/0/2/2
15	BCR	B	841	-	-	0/29/63/63	0/2/2/2
15	BCR	B	842	-	-	0/29/63/63	0/2/2/2
15	BCR	B	843	-	-	0/29/63/63	0/2/2/2
15	BCR	B	844	-	-	0/18/35/63	0/1/1/2
15	BCR	B	845	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	B	846	-	-	0/29/63/63	0/2/2/2
15	BCR	B	847	-	-	0/29/63/63	0/2/2/2
18	LMG	B	848	-	-	0/50/70/70	0/1/1/1
15	BCR	B	849	-	-	0/29/63/63	0/2/2/2
15	BCR	B	850	-	-	0/29/63/63	0/2/2/2
17	SF4	C	101	3	-	0/0/48/48	0/0/5/5
17	SF4	C	102	3	-	0/0/48/48	0/0/5/5
13	CLA	F	1301	-	-	0/11/111/135	0/0/9/9
15	BCR	F	1302	-	-	0/29/63/63	0/2/2/2
13	CLA	I	101	-	-	0/37/135/135	0/0/9/9
15	BCR	I	102	-	-	0/29/63/63	0/2/2/2
13	CLA	J	1101	-	-	0/37/135/135	0/0/9/9
13	CLA	J	1102	8	-	0/11/111/135	0/0/9/9
13	CLA	J	1103	-	-	0/2/96/135	0/0/9/9
15	BCR	J	1104	-	-	0/29/63/63	0/2/2/2
15	BCR	J	1105	-	-	0/29/63/63	0/2/2/2
13	CLA	L	1002	10	-	0/37/135/135	0/0/9/9
13	CLA	L	1003	-	-	0/37/135/135	0/0/9/9
13	CLA	L	1004	-	-	0/37/135/135	0/0/9/9
15	BCR	L	1005	-	-	0/29/63/63	0/2/2/2
15	BCR	L	1006	-	-	0/29/63/63	0/2/2/2
13	CLA	M	1201	-	-	0/23/122/135	0/0/9/9
13	CLA	M	1202	-	-	0/11/111/135	0/0/9/9
15	BCR	M	1203	-	-	0/29/63/63	0/2/2/2
16	LHG	X	101	-	-	0/26/26/53	0/0/0/0
13	CLA	X	102	12	-	0/11/111/135	0/0/9/9

All (1826) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	856	SF4	S3-FE4	-21.72	2.18	2.33
17	C	101	SF4	S2-FE1	-21.57	2.18	2.33
17	A	856	SF4	S1-FE4	-21.53	2.18	2.33
17	C	102	SF4	S3-FE2	-21.39	2.18	2.33
17	C	102	SF4	S4-FE3	-21.37	2.18	2.33
17	C	101	SF4	S4-FE1	-21.27	2.18	2.33
17	A	856	SF4	S2-FE3	-21.26	2.19	2.33
17	C	102	SF4	S1-FE4	-21.18	2.19	2.33
17	C	101	SF4	S2-FE4	-21.15	2.19	2.33
17	C	102	SF4	S1-FE2	-21.09	2.19	2.33
17	C	101	SF4	S3-FE1	-21.06	2.19	2.33
17	A	856	SF4	S3-FE2	-21.03	2.19	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	856	SF4	S2-FE4	-21.02	2.19	2.33
17	C	102	SF4	S4-FE2	-21.00	2.19	2.33
17	C	101	SF4	S3-FE4	-21.00	2.19	2.33
17	C	101	SF4	S4-FE2	-20.97	2.19	2.33
17	C	102	SF4	S2-FE3	-20.97	2.19	2.33
17	A	856	SF4	S2-FE1	-20.96	2.19	2.33
17	A	856	SF4	S4-FE1	-20.96	2.19	2.33
17	C	102	SF4	S4-FE1	-20.96	2.19	2.33
17	C	101	SF4	S4-FE3	-20.86	2.19	2.33
17	A	856	SF4	S1-FE3	-20.85	2.19	2.33
17	C	101	SF4	S3-FE2	-20.84	2.19	2.33
17	A	856	SF4	S3-FE1	-20.79	2.19	2.33
17	A	856	SF4	S4-FE3	-20.75	2.19	2.33
17	C	101	SF4	S1-FE4	-20.75	2.19	2.33
17	C	101	SF4	S1-FE2	-20.71	2.19	2.33
17	A	856	SF4	S4-FE2	-20.69	2.19	2.33
17	A	856	SF4	S1-FE2	-20.63	2.19	2.33
17	C	101	SF4	S2-FE3	-20.60	2.19	2.33
17	C	101	SF4	S1-FE3	-20.59	2.19	2.33
17	C	102	SF4	S2-FE1	-20.53	2.19	2.33
17	C	102	SF4	S1-FE3	-20.48	2.19	2.33
17	C	102	SF4	S2-FE4	-20.38	2.19	2.33
17	C	102	SF4	S3-FE4	-20.35	2.19	2.33
17	C	102	SF4	S3-FE1	-20.26	2.19	2.33
13	J	1103	CLA	CBD-CHA	16.20	1.55	1.41
13	A	844	CLA	CBD-CHA	16.18	1.55	1.41
16	A	854	LHG	C25-C24	-14.43	1.49	1.55
16	X	101	LHG	C10-C9	-14.21	1.49	1.55
16	A	854	LHG	C13-C12	-13.72	1.49	1.55
13	A	844	CLA	CBD-CAD	7.38	1.47	1.41
13	F	1301	CLA	CBA-CGA	7.27	1.54	1.49
13	B	810	CLA	CBA-CGA	7.18	1.54	1.49
13	J	1103	CLA	CBD-CAD	6.86	1.47	1.41
13	M	1202	CLA	CBA-CGA	6.86	1.53	1.49
13	B	819	CLA	CBA-CGA	6.54	1.53	1.49
13	X	102	CLA	CBA-CGA	6.54	1.53	1.49
13	B	821	CLA	CBA-CGA	6.37	1.53	1.49
13	B	828	CLA	CBA-CGA	6.35	1.53	1.49
13	J	1102	CLA	CBA-CGA	6.24	1.53	1.49
13	B	813	CLA	CBA-CGA	6.16	1.53	1.49
13	B	834	CLA	CBA-CGA	6.12	1.53	1.49
13	A	815	CLA	CBA-CGA	6.04	1.53	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	855	CLA	CBA-CGA	6.00	1.53	1.49
13	A	810	CLA	CBA-CGA	6.00	1.53	1.49
13	A	844	CLA	CBA-CGA	5.99	1.53	1.49
13	A	836	CLA	CBA-CGA	5.95	1.53	1.49
13	B	833	CLA	CBA-CGA	5.91	1.53	1.49
13	B	832	CLA	CBA-CGA	5.61	1.53	1.49
13	A	814	CLA	CBA-CGA	5.51	1.53	1.49
13	B	809	CLA	CBA-CGA	5.33	1.52	1.49
13	A	823	CLA	C6-C5	-4.96	1.53	1.55
13	A	820	CLA	C16-C15	-4.85	1.53	1.55
13	A	837	CLA	C6-C5	-4.83	1.53	1.55
13	A	841	CLA	C6-C5	-4.78	1.53	1.55
15	B	844	BCR	C14-C13	4.67	1.39	1.33
14	A	846	PQN	C12-C13	4.45	1.41	1.32
13	B	811	CLA	C2-C3	4.28	1.41	1.32
13	A	807	CLA	C6-C5	-4.24	1.53	1.55
14	B	840	PQN	C12-C13	4.22	1.41	1.32
13	A	825	CLA	C2-C3	4.05	1.41	1.32
13	A	805	CLA	C2-C3	4.05	1.41	1.32
13	A	826	CLA	C2-C3	4.04	1.41	1.32
13	A	832	CLA	C2-C3	4.00	1.41	1.32
13	A	842	CLA	C2-C3	3.98	1.41	1.32
13	B	826	CLA	C2-C3	3.98	1.41	1.32
13	A	808	CLA	C2-C3	3.98	1.41	1.32
13	B	827	CLA	C2-C3	3.97	1.41	1.32
13	B	835	CLA	C2-C3	3.95	1.40	1.32
13	A	837	CLA	C2-C3	3.93	1.40	1.32
13	A	809	CLA	C2-C3	3.93	1.40	1.32
13	A	811	CLA	C2-C3	3.92	1.40	1.32
13	A	835	CLA	C2-C3	3.92	1.40	1.32
13	M	1201	CLA	C2-C3	3.91	1.40	1.32
13	A	801	CLA	C2-C3	3.91	1.40	1.32
13	B	830	CLA	C2-C3	3.90	1.40	1.32
13	A	804	CLA	C2-C3	3.88	1.40	1.32
13	A	834	CLA	C2-C3	3.88	1.40	1.32
13	B	815	CLA	C2-C3	3.88	1.40	1.32
13	B	822	CLA	C2-C3	3.88	1.40	1.32
13	B	831	CLA	C2-C3	3.88	1.40	1.32
13	B	824	CLA	C2-C3	3.87	1.40	1.32
13	A	830	CLA	C2-C3	3.88	1.40	1.32
13	B	836	CLA	C2-C3	3.85	1.40	1.32
13	A	817	CLA	C2-C3	3.85	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	814	CLA	C2-C3	3.84	1.40	1.32
13	B	839	CLA	C2-C3	3.85	1.40	1.32
13	A	821	CLA	C2-C3	3.84	1.40	1.32
13	B	838	CLA	C2-C3	3.84	1.40	1.32
13	A	840	CLA	C2-C3	3.83	1.40	1.32
13	A	833	CLA	C2-C3	3.82	1.40	1.32
13	A	824	CLA	C2-C3	3.81	1.40	1.32
13	A	827	CLA	C2-C3	3.81	1.40	1.32
13	A	845	CLA	C2-C3	3.80	1.40	1.32
13	A	802	CLA	C2-C3	3.79	1.40	1.32
13	A	838	CLA	C2-C3	3.80	1.40	1.32
13	A	829	CLA	C2-C3	3.79	1.40	1.32
13	J	1101	CLA	C2-C3	3.79	1.40	1.32
13	B	805	CLA	C2-C3	3.79	1.40	1.32
13	B	825	CLA	C2-C3	3.78	1.40	1.32
13	L	1003	CLA	C2-C3	3.79	1.40	1.32
13	B	803	CLA	C2-C3	3.78	1.40	1.32
13	L	1002	CLA	C2-C3	3.77	1.40	1.32
13	A	837	CLA	C5-C3	3.76	1.56	1.51
13	B	808	CLA	C2-C3	3.75	1.40	1.32
13	A	812	CLA	C2-C3	3.75	1.40	1.32
13	A	841	CLA	C2-C3	3.75	1.40	1.32
13	A	820	CLA	C2-C3	3.75	1.40	1.32
13	I	101	CLA	C2-C3	3.74	1.40	1.32
13	A	813	CLA	C2-C3	3.74	1.40	1.32
13	A	823	CLA	C2-C3	3.73	1.40	1.32
13	B	817	CLA	C2-C3	3.73	1.40	1.32
13	A	841	CLA	C5-C3	3.72	1.56	1.51
13	B	801	CLA	C2-C3	3.71	1.40	1.32
13	A	828	CLA	C2-C3	3.69	1.40	1.32
15	A	852	BCR	C20-C21	3.69	1.54	1.43
13	L	1004	CLA	C2-C3	3.69	1.40	1.32
13	B	802	CLA	C2-C3	3.68	1.40	1.32
13	B	816	CLA	C2-C3	3.67	1.40	1.32
13	A	803	CLA	C2-C3	3.66	1.40	1.32
13	A	807	CLA	C5-C3	3.65	1.56	1.51
13	B	807	CLA	C2-C3	3.65	1.40	1.32
13	B	812	CLA	C2-C3	3.65	1.40	1.32
13	B	806	CLA	C2-C3	3.64	1.40	1.32
13	A	819	CLA	C2-C3	3.64	1.40	1.32
15	A	852	BCR	C21-C22	3.61	1.40	1.35
13	A	824	CLA	C1B-CHB	-3.61	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	850	BCR	C20-C21	3.61	1.54	1.43
15	B	842	BCR	C20-C21	3.61	1.54	1.43
13	B	804	CLA	C2-C3	3.61	1.40	1.32
13	A	806	CLA	C2-C3	3.60	1.40	1.32
15	B	844	BCR	C20-C21	3.60	1.54	1.43
13	A	823	CLA	C5-C3	3.59	1.56	1.51
15	A	850	BCR	C17-C18	3.58	1.40	1.35
15	A	848	BCR	C20-C21	3.58	1.54	1.43
15	A	851	BCR	C20-C21	3.58	1.54	1.43
13	A	818	CLA	C2-C3	3.57	1.40	1.32
13	A	834	CLA	C1B-CHB	-3.57	1.30	1.39
15	J	1105	BCR	C20-C21	3.57	1.54	1.43
15	L	1005	BCR	C20-C21	3.56	1.54	1.43
15	B	844	BCR	C17-C18	3.56	1.40	1.35
15	B	850	BCR	C20-C21	3.55	1.54	1.43
15	B	845	BCR	C20-C21	3.54	1.54	1.43
13	B	816	CLA	C1B-CHB	-3.54	1.30	1.39
13	B	820	CLA	C2-C3	3.54	1.40	1.32
13	A	808	CLA	MG-ND	-3.54	1.97	2.05
13	A	843	CLA	C2-C3	3.54	1.40	1.32
15	L	1006	BCR	C20-C21	3.53	1.54	1.43
13	L	1002	CLA	C1B-CHB	-3.53	1.30	1.39
15	J	1104	BCR	C20-C21	3.51	1.54	1.43
13	A	801	CLA	C1B-CHB	-3.50	1.30	1.39
15	M	1203	BCR	C20-C21	3.50	1.54	1.43
13	B	801	CLA	C1B-CHB	-3.49	1.30	1.39
13	A	822	CLA	C1B-CHB	-3.49	1.30	1.39
13	A	802	CLA	C1B-CHB	-3.48	1.30	1.39
13	B	803	CLA	C1B-CHB	-3.48	1.30	1.39
15	B	847	BCR	C20-C21	3.48	1.54	1.43
13	B	802	CLA	MG-ND	-3.48	1.97	2.05
13	B	828	CLA	C1B-CHB	-3.48	1.30	1.39
13	A	835	CLA	C1B-CHB	-3.48	1.30	1.39
15	B	846	BCR	C20-C21	3.47	1.54	1.43
16	A	854	LHG	O7-C5	-3.46	1.37	1.46
16	X	101	LHG	O7-C5	-3.46	1.37	1.46
15	A	850	BCR	C23-C22	3.46	1.53	1.45
15	A	847	BCR	C20-C21	3.46	1.54	1.43
13	B	804	CLA	C1B-CHB	-3.45	1.30	1.39
13	L	1003	CLA	C1B-CHB	-3.45	1.30	1.39
13	B	835	CLA	MG-ND	-3.44	1.97	2.05
13	B	822	CLA	MG-ND	-3.44	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	102	CLA	MG-ND	-3.44	1.97	2.05
13	B	821	CLA	C1B-CHB	-3.44	1.30	1.39
13	A	831	CLA	C1B-CHB	-3.44	1.30	1.39
13	B	818	CLA	C1B-CHB	-3.44	1.30	1.39
15	B	849	BCR	C20-C21	3.44	1.54	1.43
13	B	825	CLA	C1B-CHB	-3.43	1.30	1.39
13	B	826	CLA	C1B-CHB	-3.43	1.30	1.39
13	B	819	CLA	C1B-CHB	-3.43	1.30	1.39
13	F	1301	CLA	MG-ND	-3.42	1.97	2.05
13	A	804	CLA	C1B-CHB	-3.42	1.30	1.39
15	A	852	BCR	C23-C22	3.42	1.53	1.45
13	B	809	CLA	C1B-CHB	-3.42	1.30	1.39
13	J	1103	CLA	C1B-CHB	-3.42	1.30	1.39
13	F	1301	CLA	C1B-CHB	-3.41	1.30	1.39
13	A	828	CLA	C1B-CHB	-3.41	1.30	1.39
15	A	852	BCR	C17-C18	3.41	1.40	1.35
13	A	803	CLA	C1B-CHB	-3.41	1.30	1.39
13	A	809	CLA	C1B-CHB	-3.41	1.30	1.39
13	A	820	CLA	C1B-CHB	-3.41	1.30	1.39
13	A	837	CLA	MG-ND	-3.41	1.97	2.05
13	A	844	CLA	CHA-C1A	-3.41	1.33	1.45
15	B	842	BCR	C23-C22	3.40	1.53	1.45
13	A	818	CLA	C1B-CHB	-3.40	1.30	1.39
13	A	815	CLA	C1B-CHB	-3.40	1.30	1.39
15	J	1104	BCR	C17-C18	3.40	1.40	1.35
15	F	1302	BCR	C20-C21	3.40	1.53	1.43
13	A	826	CLA	C1B-CHB	-3.39	1.30	1.39
13	A	810	CLA	C1B-CHB	-3.39	1.30	1.39
13	B	810	CLA	C1B-CHB	-3.39	1.30	1.39
13	B	829	CLA	C1B-CHB	-3.38	1.30	1.39
13	B	813	CLA	MG-ND	-3.38	1.97	2.05
15	B	843	BCR	C20-C21	3.38	1.53	1.43
15	J	1105	BCR	C23-C22	3.38	1.53	1.45
15	B	841	BCR	C20-C21	3.38	1.53	1.43
13	A	837	CLA	C1B-CHB	-3.38	1.30	1.39
15	B	847	BCR	C17-C18	3.38	1.40	1.35
13	X	102	CLA	C1B-CHB	-3.37	1.30	1.39
13	A	836	CLA	C1B-CHB	-3.37	1.30	1.39
13	A	836	CLA	MG-ND	-3.37	1.97	2.05
13	B	808	CLA	MG-ND	-3.36	1.97	2.05
13	A	811	CLA	C1B-CHB	-3.36	1.30	1.39
13	A	807	CLA	C2-C3	3.36	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	802	CLA	C1B-CHB	-3.36	1.30	1.39
15	J	1105	BCR	C17-C18	3.36	1.40	1.35
13	A	842	CLA	MG-ND	-3.35	1.97	2.05
15	A	848	BCR	C17-C18	3.35	1.40	1.35
15	B	845	BCR	C23-C22	3.35	1.53	1.45
13	B	837	CLA	C1B-CHB	-3.35	1.30	1.39
13	B	813	CLA	C1B-CHB	-3.35	1.30	1.39
13	A	817	CLA	C1B-CHB	-3.35	1.30	1.39
13	B	830	CLA	C1B-CHB	-3.34	1.30	1.39
15	J	1104	BCR	C23-C22	3.34	1.53	1.45
13	A	814	CLA	C1B-CHB	-3.34	1.30	1.39
13	A	838	CLA	C1B-CHB	-3.34	1.30	1.39
13	B	807	CLA	C1B-CHB	-3.34	1.30	1.39
15	A	848	BCR	C23-C22	3.34	1.53	1.45
13	B	832	CLA	C1B-CHB	-3.34	1.30	1.39
13	A	822	CLA	MG-ND	-3.34	1.97	2.05
13	B	823	CLA	MG-ND	-3.33	1.97	2.05
13	B	839	CLA	C1B-CHB	-3.33	1.30	1.39
15	B	842	BCR	C17-C18	3.33	1.40	1.35
13	A	839	CLA	C1B-CHB	-3.33	1.30	1.39
13	A	805	CLA	C1B-CHB	-3.32	1.30	1.39
13	B	827	CLA	C1B-CHB	-3.32	1.30	1.39
13	A	833	CLA	C1B-CHB	-3.32	1.30	1.39
15	B	847	BCR	C23-C22	3.32	1.53	1.45
13	J	1103	CLA	CHA-C1A	-3.32	1.33	1.45
13	B	812	CLA	MG-ND	-3.32	1.97	2.05
13	B	823	CLA	C1B-CHB	-3.32	1.30	1.39
13	B	822	CLA	C1B-CHB	-3.31	1.30	1.39
13	A	845	CLA	C1B-CHB	-3.31	1.30	1.39
13	A	813	CLA	C1B-CHB	-3.31	1.30	1.39
13	A	838	CLA	MG-ND	-3.30	1.97	2.05
13	I	101	CLA	C1B-CHB	-3.31	1.30	1.39
13	A	819	CLA	C1B-CHB	-3.31	1.30	1.39
13	A	808	CLA	C1B-CHB	-3.30	1.30	1.39
13	B	833	CLA	MG-ND	-3.30	1.97	2.05
13	B	807	CLA	MG-ND	-3.30	1.97	2.05
13	B	806	CLA	C1B-CHB	-3.30	1.30	1.39
15	I	102	BCR	C20-C21	3.30	1.53	1.43
13	B	811	CLA	MG-ND	-3.29	1.97	2.05
13	B	835	CLA	O2D-CED	-3.29	1.37	1.45
13	A	816	CLA	C1B-CHB	-3.29	1.30	1.39
15	B	846	BCR	C23-C22	3.29	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	855	CLA	C1B-CHB	-3.29	1.30	1.39
13	B	833	CLA	C1B-CHB	-3.29	1.30	1.39
13	B	818	CLA	MG-ND	-3.29	1.97	2.05
13	A	842	CLA	C1B-CHB	-3.29	1.30	1.39
13	A	824	CLA	MG-ND	-3.29	1.97	2.05
13	B	811	CLA	C1B-CHB	-3.29	1.30	1.39
15	M	1203	BCR	C17-C18	3.29	1.40	1.35
15	B	850	BCR	C17-C18	3.28	1.40	1.35
15	A	849	BCR	C20-C21	3.28	1.53	1.43
13	A	826	CLA	MG-ND	-3.28	1.97	2.05
13	J	1101	CLA	MG-ND	-3.28	1.97	2.05
13	B	828	CLA	MG-ND	-3.28	1.97	2.05
13	J	1102	CLA	C1B-CHB	-3.28	1.30	1.39
13	A	825	CLA	C1B-CHB	-3.28	1.30	1.39
13	B	817	CLA	C1B-CHB	-3.28	1.30	1.39
13	A	834	CLA	MG-ND	-3.28	1.97	2.05
13	A	844	CLA	C1B-CHB	-3.27	1.30	1.39
15	B	844	BCR	C21-C22	3.27	1.40	1.35
13	M	1201	CLA	C1B-CHB	-3.27	1.30	1.39
13	B	815	CLA	C1B-CHB	-3.27	1.30	1.39
15	A	850	BCR	C11-C10	3.27	1.53	1.43
13	B	834	CLA	C1B-CHB	-3.27	1.30	1.39
13	B	825	CLA	MG-ND	-3.27	1.97	2.05
13	A	802	CLA	MG-ND	-3.27	1.97	2.05
13	A	827	CLA	MG-ND	-3.27	1.97	2.05
13	A	855	CLA	MG-ND	-3.27	1.97	2.05
13	B	824	CLA	MG-ND	-3.26	1.97	2.05
13	B	824	CLA	C1B-CHB	-3.26	1.30	1.39
13	A	841	CLA	MG-ND	-3.26	1.97	2.05
13	B	831	CLA	C1B-CHB	-3.26	1.30	1.39
13	L	1004	CLA	C1B-CHB	-3.26	1.30	1.39
15	A	851	BCR	C21-C22	3.26	1.40	1.35
13	B	808	CLA	C1B-CHB	-3.26	1.30	1.39
15	M	1203	BCR	C23-C22	3.26	1.53	1.45
13	A	829	CLA	C1B-CHB	-3.26	1.30	1.39
15	B	844	BCR	C15-C14	3.26	1.53	1.43
15	B	842	BCR	C15-C14	3.26	1.53	1.43
13	M	1202	CLA	C1B-CHB	-3.25	1.30	1.39
15	F	1302	BCR	C17-C18	3.25	1.40	1.35
13	B	836	CLA	MG-ND	-3.25	1.97	2.05
15	B	844	BCR	C23-C22	3.25	1.53	1.45
15	A	847	BCR	C23-C22	3.25	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	838	CLA	C1B-CHB	-3.25	1.30	1.39
13	J	1103	CLA	C3D-CAD	-3.24	1.44	1.49
13	A	807	CLA	C1B-CHB	-3.24	1.30	1.39
15	L	1006	BCR	C23-C22	3.24	1.53	1.45
13	I	101	CLA	MG-ND	-3.24	1.97	2.05
13	B	836	CLA	C1B-CHB	-3.24	1.30	1.39
13	A	825	CLA	MG-ND	-3.24	1.97	2.05
13	A	806	CLA	C1B-CHB	-3.24	1.30	1.39
13	B	814	CLA	C1B-CHB	-3.24	1.30	1.39
15	B	845	BCR	C21-C22	3.24	1.40	1.35
13	A	814	CLA	MG-ND	-3.24	1.97	2.05
13	A	813	CLA	MG-ND	-3.24	1.97	2.05
15	L	1006	BCR	C15-C14	3.24	1.53	1.43
16	A	853	LHG	O7-C5	-3.24	1.38	1.46
13	A	823	CLA	C1B-CHB	-3.24	1.30	1.39
15	A	852	BCR	C16-C17	3.24	1.53	1.43
13	B	838	CLA	MG-ND	-3.24	1.97	2.05
15	A	847	BCR	C17-C18	3.23	1.40	1.35
13	B	834	CLA	MG-ND	-3.23	1.97	2.05
15	B	843	BCR	C17-C18	3.23	1.40	1.35
13	B	831	CLA	MG-ND	-3.23	1.97	2.05
13	A	841	CLA	C1B-CHB	-3.23	1.30	1.39
15	A	847	BCR	C15-C14	3.23	1.53	1.43
13	J	1101	CLA	C1B-CHB	-3.23	1.31	1.39
13	B	812	CLA	C1B-CHB	-3.23	1.31	1.39
13	B	820	CLA	C1B-CHB	-3.23	1.31	1.39
13	A	821	CLA	C1B-CHB	-3.22	1.31	1.39
15	A	850	BCR	C21-C22	3.22	1.40	1.35
15	F	1302	BCR	C15-C14	3.22	1.53	1.43
13	A	812	CLA	MG-ND	-3.22	1.97	2.05
15	B	847	BCR	C15-C14	3.22	1.53	1.43
15	A	851	BCR	C23-C22	3.22	1.53	1.45
13	J	1102	CLA	MG-ND	-3.22	1.97	2.05
13	A	833	CLA	MG-ND	-3.22	1.97	2.05
13	B	806	CLA	MG-ND	-3.22	1.97	2.05
13	A	843	CLA	C1B-CHB	-3.21	1.31	1.39
15	A	848	BCR	C15-C14	3.21	1.53	1.43
15	A	850	BCR	C15-C14	3.21	1.53	1.43
13	B	816	CLA	MG-ND	-3.21	1.97	2.05
13	B	817	CLA	MG-ND	-3.21	1.97	2.05
15	I	102	BCR	C17-C18	3.21	1.40	1.35
15	L	1005	BCR	C17-C18	3.21	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	827	CLA	C1B-CHB	-3.21	1.31	1.39
13	A	830	CLA	C1B-CHB	-3.21	1.31	1.39
13	B	805	CLA	C1B-CHB	-3.21	1.31	1.39
13	M	1202	CLA	MG-ND	-3.20	1.97	2.05
13	L	1002	CLA	MG-ND	-3.20	1.97	2.05
15	B	841	BCR	C23-C22	3.20	1.53	1.45
15	B	842	BCR	C16-C17	3.20	1.53	1.43
15	B	850	BCR	C11-C10	3.20	1.53	1.43
15	B	841	BCR	C17-C18	3.20	1.40	1.35
15	B	841	BCR	C26-C25	3.20	1.39	1.34
13	L	1004	CLA	MG-ND	-3.20	1.97	2.05
15	A	852	BCR	C19-C18	3.20	1.53	1.45
13	B	820	CLA	MG-ND	-3.20	1.97	2.05
13	A	809	CLA	MG-ND	-3.20	1.97	2.05
15	J	1104	BCR	C11-C10	3.19	1.53	1.43
13	B	835	CLA	C1B-CHB	-3.19	1.31	1.39
15	B	850	BCR	C23-C22	3.19	1.53	1.45
13	A	803	CLA	MG-ND	-3.19	1.98	2.05
13	A	815	CLA	MG-ND	-3.18	1.98	2.05
15	J	1104	BCR	C15-C14	3.18	1.53	1.43
13	B	821	CLA	MG-ND	-3.18	1.98	2.05
15	B	844	BCR	C16-C17	3.18	1.53	1.43
13	B	803	CLA	MG-ND	-3.18	1.98	2.05
13	L	1003	CLA	MG-ND	-3.18	1.98	2.05
15	J	1105	BCR	C15-C14	3.18	1.53	1.43
13	A	820	CLA	MG-ND	-3.18	1.98	2.05
13	A	843	CLA	MG-ND	-3.18	1.98	2.05
15	B	846	BCR	C15-C14	3.17	1.53	1.43
13	A	812	CLA	C1B-CHB	-3.17	1.31	1.39
13	A	816	CLA	MG-ND	-3.16	1.98	2.05
15	A	850	BCR	C16-C17	3.16	1.53	1.43
15	B	843	BCR	C15-C14	3.16	1.53	1.43
13	A	837	CLA	O2D-CED	-3.16	1.37	1.45
13	A	840	CLA	C1B-CHB	-3.15	1.31	1.39
15	L	1005	BCR	C23-C22	3.15	1.52	1.45
13	A	831	CLA	MG-ND	-3.15	1.98	2.05
15	A	851	BCR	C17-C18	3.15	1.39	1.35
15	L	1006	BCR	C17-C18	3.15	1.39	1.35
13	B	819	CLA	MG-ND	-3.15	1.98	2.05
15	A	847	BCR	C26-C25	3.14	1.39	1.34
15	F	1302	BCR	C16-C17	3.14	1.53	1.43
15	L	1005	BCR	C11-C10	3.15	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	811	CLA	MG-ND	-3.14	1.98	2.05
15	B	842	BCR	C8-C9	3.14	1.52	1.45
13	A	806	CLA	MG-ND	-3.14	1.98	2.05
15	B	849	BCR	C15-C14	3.14	1.53	1.43
15	B	841	BCR	C15-C14	3.14	1.53	1.43
15	J	1104	BCR	C8-C9	3.14	1.52	1.45
15	A	848	BCR	C21-C22	3.14	1.39	1.35
15	B	849	BCR	C23-C22	3.14	1.52	1.45
13	A	840	CLA	C1C-C2C	3.13	1.51	1.44
15	L	1006	BCR	C5-C6	3.14	1.39	1.34
13	A	821	CLA	MG-ND	-3.13	1.98	2.05
15	A	848	BCR	C11-C10	3.14	1.53	1.43
15	J	1104	BCR	C16-C17	3.13	1.53	1.43
13	A	818	CLA	MG-ND	-3.13	1.98	2.05
15	L	1006	BCR	C11-C10	3.13	1.53	1.43
13	A	832	CLA	MG-ND	-3.13	1.98	2.05
15	B	845	BCR	C17-C18	3.13	1.39	1.35
13	B	815	CLA	MG-ND	-3.12	1.98	2.05
13	A	832	CLA	C1B-CHB	-3.12	1.31	1.39
15	B	843	BCR	C11-C10	3.12	1.53	1.43
15	A	852	BCR	C15-C14	3.12	1.53	1.43
15	A	847	BCR	C16-C17	3.12	1.53	1.43
15	A	851	BCR	C15-C14	3.12	1.53	1.43
13	B	827	CLA	C1C-C2C	3.12	1.51	1.44
15	B	842	BCR	C11-C10	3.12	1.53	1.43
15	J	1105	BCR	C21-C22	3.12	1.39	1.35
13	B	832	CLA	MG-ND	-3.12	1.98	2.05
15	B	841	BCR	C11-C10	3.11	1.53	1.43
15	A	847	BCR	C11-C10	3.11	1.53	1.43
15	M	1203	BCR	C15-C14	3.11	1.53	1.43
13	B	837	CLA	MG-ND	-3.11	1.98	2.05
15	B	850	BCR	C21-C22	3.11	1.39	1.35
13	A	835	CLA	MG-ND	-3.11	1.98	2.05
15	B	850	BCR	C15-C14	3.11	1.53	1.43
13	B	810	CLA	MG-ND	-3.11	1.98	2.05
15	B	847	BCR	C16-C17	3.11	1.53	1.43
15	B	846	BCR	C17-C18	3.10	1.39	1.35
15	B	849	BCR	C21-C22	3.10	1.39	1.35
16	A	854	LHG	O8-C6	-3.10	1.37	1.45
15	A	849	BCR	C23-C22	3.10	1.52	1.45
13	A	814	CLA	O2D-CED	-3.10	1.37	1.45
15	A	847	BCR	C8-C9	3.10	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	848	BCR	C16-C17	3.09	1.52	1.43
15	L	1005	BCR	C15-C14	3.09	1.52	1.43
15	A	850	BCR	C26-C25	3.09	1.39	1.34
13	A	801	CLA	MG-ND	-3.08	1.98	2.05
15	J	1105	BCR	C16-C17	3.08	1.52	1.43
13	A	804	CLA	MG-ND	-3.08	1.98	2.05
13	B	838	CLA	C1C-C2C	3.08	1.50	1.44
15	B	846	BCR	C21-C22	3.08	1.39	1.35
15	F	1302	BCR	C23-C22	3.08	1.52	1.45
15	B	841	BCR	C16-C17	3.07	1.52	1.43
15	A	850	BCR	C12-C13	3.07	1.52	1.45
15	B	846	BCR	C26-C25	3.07	1.39	1.34
15	L	1006	BCR	C16-C17	3.07	1.52	1.43
15	B	847	BCR	C11-C10	3.07	1.52	1.43
15	A	850	BCR	C19-C18	3.07	1.52	1.45
13	B	809	CLA	MG-ND	-3.07	1.98	2.05
15	B	841	BCR	C8-C9	3.07	1.52	1.45
15	J	1105	BCR	C11-C10	3.07	1.52	1.43
13	B	805	CLA	C4C-C3C	3.07	1.50	1.45
15	B	842	BCR	C21-C22	3.06	1.39	1.35
15	I	102	BCR	C15-C14	3.06	1.52	1.43
15	B	849	BCR	C16-C17	3.07	1.52	1.43
15	B	850	BCR	C16-C17	3.06	1.52	1.43
13	A	814	CLA	C1C-C2C	3.06	1.50	1.44
15	B	842	BCR	C26-C25	3.06	1.39	1.34
15	B	850	BCR	C8-C9	3.06	1.52	1.45
13	A	807	CLA	C1C-C2C	3.06	1.50	1.44
15	M	1203	BCR	C16-C17	3.06	1.52	1.43
15	A	851	BCR	C11-C10	3.06	1.52	1.43
15	B	849	BCR	C17-C18	3.06	1.39	1.35
15	A	847	BCR	C14-C13	3.05	1.39	1.35
13	A	820	CLA	C4A-NA	-3.06	1.32	1.39
13	A	807	CLA	O2D-CGD	3.06	1.41	1.33
13	A	819	CLA	MG-ND	-3.06	1.98	2.05
13	A	844	CLA	MG-ND	-3.06	1.98	2.05
13	B	826	CLA	O2D-CED	-3.05	1.37	1.45
13	B	837	CLA	O2A-C1	-3.05	1.41	1.45
15	M	1203	BCR	C21-C22	3.05	1.39	1.35
15	B	845	BCR	C15-C14	3.05	1.52	1.43
15	B	846	BCR	C11-C10	3.05	1.52	1.43
15	F	1302	BCR	C26-C25	3.05	1.39	1.34
15	B	849	BCR	C26-C25	3.05	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	845	CLA	C7-C6	-3.04	1.53	1.55
15	B	843	BCR	C16-C17	3.04	1.52	1.43
16	X	101	LHG	O8-C6	-3.04	1.38	1.45
15	F	1302	BCR	C11-C10	3.04	1.52	1.43
13	B	832	CLA	C1C-C2C	3.04	1.50	1.44
15	B	846	BCR	C16-C17	3.04	1.52	1.43
15	A	848	BCR	C14-C13	3.04	1.39	1.35
15	B	845	BCR	C16-C17	3.04	1.52	1.43
15	A	851	BCR	C8-C9	3.04	1.52	1.45
15	A	851	BCR	C16-C17	3.04	1.52	1.43
15	B	844	BCR	C19-C18	3.04	1.52	1.45
13	A	829	CLA	MG-ND	-3.03	1.98	2.05
13	B	807	CLA	C1C-C2C	3.03	1.50	1.44
13	B	805	CLA	MG-ND	-3.03	1.98	2.05
15	B	842	BCR	C19-C18	3.03	1.52	1.45
15	B	842	BCR	C14-C13	3.03	1.39	1.35
13	B	802	CLA	C1C-C2C	3.02	1.50	1.44
15	A	852	BCR	C11-C10	3.02	1.52	1.43
15	A	848	BCR	C19-C18	3.02	1.52	1.45
13	A	802	CLA	C4A-NA	-3.01	1.32	1.39
13	A	807	CLA	MG-ND	-3.01	1.98	2.05
15	J	1104	BCR	C21-C22	3.01	1.39	1.35
13	B	808	CLA	C1C-C2C	3.01	1.50	1.44
15	J	1104	BCR	C19-C18	3.01	1.52	1.45
13	A	808	CLA	C1C-C2C	3.01	1.50	1.44
15	M	1203	BCR	C11-C10	3.01	1.52	1.43
13	M	1201	CLA	MG-ND	-3.01	1.98	2.05
13	B	801	CLA	MG-ND	-3.01	1.98	2.05
13	B	801	CLA	C4A-NA	-3.00	1.32	1.39
15	B	846	BCR	C14-C13	3.00	1.39	1.35
13	B	811	CLA	C1C-C2C	3.00	1.50	1.44
13	L	1002	CLA	C1C-C2C	3.00	1.50	1.44
15	A	848	BCR	C8-C9	3.00	1.52	1.45
13	A	832	CLA	O2A-CGA	3.00	1.42	1.33
13	A	837	CLA	O2A-CGA	3.00	1.42	1.33
13	A	809	CLA	C1C-C2C	3.00	1.50	1.44
13	A	839	CLA	C1C-C2C	3.00	1.50	1.44
15	A	849	BCR	C15-C14	3.00	1.52	1.43
13	A	844	CLA	C1C-C2C	3.00	1.50	1.44
15	I	102	BCR	C16-C17	3.00	1.52	1.43
15	B	846	BCR	C8-C9	2.99	1.52	1.45
13	B	825	CLA	C1C-C2C	2.99	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	844	CLA	C4A-NA	-2.99	1.32	1.39
13	A	822	CLA	C4-C3	2.99	1.52	1.47
13	B	816	CLA	C4A-NA	-2.99	1.32	1.39
13	A	826	CLA	C1C-C2C	2.99	1.50	1.44
13	A	813	CLA	C1C-C2C	2.99	1.50	1.44
13	B	839	CLA	MG-ND	-2.99	1.98	2.05
13	B	829	CLA	C4-C3	2.99	1.52	1.47
15	I	102	BCR	C23-C22	2.99	1.52	1.45
13	L	1003	CLA	C4A-NA	-2.99	1.32	1.39
13	A	828	CLA	C1C-C2C	2.99	1.50	1.44
13	B	811	CLA	O2A-CGA	2.99	1.42	1.33
13	F	1301	CLA	C1C-C2C	2.99	1.50	1.44
13	A	804	CLA	C1C-C2C	2.99	1.50	1.44
13	A	828	CLA	MG-ND	-2.98	1.98	2.05
15	A	852	BCR	C14-C13	2.98	1.39	1.35
13	A	845	CLA	MG-ND	-2.98	1.98	2.05
13	A	823	CLA	MG-ND	-2.98	1.98	2.05
15	L	1006	BCR	C21-C22	2.98	1.39	1.35
13	B	826	CLA	MG-ND	-2.98	1.98	2.05
13	M	1202	CLA	C1C-C2C	2.98	1.50	1.44
15	B	845	BCR	C8-C9	2.98	1.52	1.45
15	A	850	BCR	C8-C9	2.98	1.52	1.45
13	A	816	CLA	C4-C3	2.98	1.52	1.47
15	B	845	BCR	C11-C10	2.98	1.52	1.43
13	A	817	CLA	MG-ND	-2.98	1.98	2.05
13	B	835	CLA	O2A-CGA	2.98	1.42	1.33
15	B	843	BCR	C19-C18	2.98	1.52	1.45
13	B	827	CLA	MG-ND	-2.97	1.98	2.05
13	B	818	CLA	C1C-C2C	2.98	1.50	1.44
15	F	1302	BCR	C8-C9	2.97	1.52	1.45
15	A	849	BCR	C11-C10	2.97	1.52	1.43
15	M	1203	BCR	C19-C18	2.97	1.52	1.45
13	A	840	CLA	MG-ND	-2.97	1.98	2.05
13	B	824	CLA	C1C-C2C	2.97	1.50	1.44
13	A	823	CLA	C1C-C2C	2.96	1.50	1.44
13	B	829	CLA	MG-ND	-2.96	1.98	2.05
13	A	844	CLA	C4C-C3C	2.96	1.50	1.45
13	M	1201	CLA	C4A-NA	-2.96	1.32	1.39
15	B	850	BCR	C19-C18	2.96	1.52	1.45
15	B	847	BCR	C26-C25	2.96	1.39	1.34
13	A	838	CLA	C1C-C2C	2.96	1.50	1.44
13	A	845	CLA	C4C-C3C	2.96	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	843	CLA	C1C-C2C	2.95	1.50	1.44
13	A	819	CLA	C4A-NA	-2.95	1.32	1.39
15	A	850	BCR	C14-C13	2.95	1.39	1.35
15	J	1105	BCR	C19-C18	2.95	1.52	1.45
13	B	837	CLA	C4A-NA	-2.95	1.32	1.39
13	A	839	CLA	O2A-C1	-2.95	1.41	1.45
15	J	1105	BCR	C8-C9	2.95	1.52	1.45
15	A	849	BCR	C17-C18	2.95	1.39	1.35
13	A	831	CLA	C2-C3	2.95	1.40	1.34
15	B	847	BCR	C8-C9	2.95	1.52	1.45
15	L	1006	BCR	C19-C18	2.95	1.52	1.45
15	B	843	BCR	C23-C22	2.95	1.52	1.45
13	B	837	CLA	C1C-C2C	2.94	1.50	1.44
15	B	850	BCR	C12-C13	2.95	1.52	1.45
15	B	843	BCR	C12-C13	2.94	1.52	1.45
13	A	832	CLA	C1C-C2C	2.94	1.50	1.44
13	A	835	CLA	C4A-NA	-2.94	1.32	1.39
15	L	1005	BCR	C19-C18	2.94	1.52	1.45
13	B	836	CLA	C1C-C2C	2.94	1.50	1.44
15	B	846	BCR	C19-C18	2.94	1.52	1.45
15	A	851	BCR	C19-C18	2.94	1.52	1.45
13	B	821	CLA	C4A-NA	-2.94	1.32	1.39
13	B	826	CLA	C4A-NA	-2.94	1.32	1.39
13	A	826	CLA	O2A-CGA	2.94	1.42	1.33
13	A	817	CLA	C1C-C2C	2.94	1.50	1.44
15	B	843	BCR	C8-C9	2.93	1.52	1.45
13	A	816	CLA	C1-C2	2.93	1.54	1.49
13	A	829	CLA	C4C-C3C	2.93	1.50	1.45
13	A	839	CLA	MG-ND	-2.93	1.98	2.05
15	L	1005	BCR	C16-C17	2.93	1.52	1.43
13	B	806	CLA	C1C-C2C	2.93	1.50	1.44
13	B	810	CLA	C4A-NA	-2.93	1.32	1.39
13	A	820	CLA	C4D-C3D	-2.93	1.38	1.41
13	A	810	CLA	MG-ND	-2.93	1.98	2.05
13	B	839	CLA	C4C-C3C	2.93	1.50	1.45
13	B	807	CLA	C4A-NA	-2.92	1.32	1.39
15	L	1005	BCR	C12-C13	2.92	1.52	1.45
15	L	1005	BCR	C26-C25	2.92	1.39	1.34
15	B	845	BCR	C19-C18	2.93	1.52	1.45
15	A	847	BCR	C21-C22	2.92	1.39	1.35
13	A	801	CLA	C4A-NA	-2.92	1.32	1.39
16	A	853	LHG	O8-C6	-2.92	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1201	CLA	C1C-C2C	2.92	1.50	1.44
13	A	855	CLA	C4A-NA	-2.92	1.32	1.39
13	A	831	CLA	O2D-CED	-2.92	1.38	1.45
15	A	849	BCR	C16-C17	2.92	1.52	1.43
13	A	806	CLA	C4C-C3C	2.91	1.50	1.45
13	A	811	CLA	C1C-C2C	2.91	1.50	1.44
13	I	101	CLA	C1C-C2C	2.91	1.50	1.44
15	I	102	BCR	C11-C10	2.92	1.52	1.43
13	J	1101	CLA	C1C-C2C	2.91	1.50	1.44
15	A	848	BCR	C26-C25	2.91	1.39	1.34
13	A	830	CLA	C1C-C2C	2.91	1.50	1.44
13	M	1201	CLA	O2A-CGA	2.91	1.42	1.33
15	L	1006	BCR	C14-C13	2.91	1.39	1.35
13	A	806	CLA	C1C-C2C	2.91	1.50	1.44
15	A	849	BCR	C26-C25	2.91	1.39	1.34
13	A	821	CLA	C1C-C2C	2.91	1.50	1.44
13	J	1103	CLA	C4C-C3C	2.91	1.50	1.45
13	B	804	CLA	MG-ND	-2.91	1.98	2.05
13	A	822	CLA	C1-C2	2.91	1.54	1.49
13	B	801	CLA	C1C-C2C	2.91	1.50	1.44
15	B	849	BCR	C11-C10	2.91	1.52	1.43
13	A	808	CLA	O2A-CGA	2.91	1.42	1.33
13	A	844	CLA	C3D-CAD	-2.90	1.44	1.49
13	B	803	CLA	C4A-NA	-2.90	1.32	1.39
13	A	831	CLA	C1C-C2C	2.90	1.50	1.44
15	M	1203	BCR	C26-C25	2.90	1.39	1.34
13	A	825	CLA	C1C-C2C	2.90	1.50	1.44
13	L	1004	CLA	C4C-C3C	2.90	1.50	1.45
13	B	833	CLA	C1C-C2C	2.90	1.50	1.44
13	B	811	CLA	C4C-C3C	2.89	1.50	1.45
15	L	1006	BCR	C26-C25	2.89	1.38	1.34
13	J	1103	CLA	C1C-C2C	2.89	1.50	1.44
13	A	836	CLA	C1C-C2C	2.89	1.50	1.44
15	A	852	BCR	C26-C25	2.89	1.38	1.34
13	A	837	CLA	C1C-C2C	2.89	1.50	1.44
13	A	813	CLA	C4C-C3C	2.89	1.50	1.45
13	L	1003	CLA	O2A-CGA	2.89	1.42	1.33
13	A	802	CLA	C4C-C3C	2.88	1.50	1.45
13	J	1102	CLA	C1C-C2C	2.88	1.50	1.44
13	A	813	CLA	C4A-NA	-2.88	1.33	1.39
13	A	841	CLA	C4C-C3C	2.88	1.50	1.45
15	B	843	BCR	C14-C13	2.88	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	829	CLA	C4A-NA	-2.88	1.33	1.39
13	A	803	CLA	C1C-C2C	2.88	1.50	1.44
13	A	821	CLA	C4A-NA	-2.88	1.33	1.39
15	A	848	BCR	C12-C13	2.88	1.52	1.45
13	J	1103	CLA	MG-ND	-2.88	1.98	2.05
15	A	847	BCR	C12-C13	2.88	1.52	1.45
13	A	823	CLA	C4A-NA	-2.88	1.33	1.39
13	B	839	CLA	C4A-NA	-2.88	1.33	1.39
15	B	847	BCR	C14-C13	2.88	1.39	1.35
13	A	824	CLA	C4C-C3C	2.88	1.50	1.45
13	A	831	CLA	C5-C3	2.88	1.56	1.40
13	B	830	CLA	C1C-C2C	2.88	1.50	1.44
15	B	847	BCR	C19-C18	2.88	1.52	1.45
13	A	805	CLA	C1C-C2C	2.88	1.50	1.44
15	J	1105	BCR	C12-C13	2.87	1.52	1.45
15	F	1302	BCR	C14-C13	2.87	1.39	1.35
13	B	825	CLA	C4A-NA	-2.87	1.33	1.39
13	A	802	CLA	O2A-CGA	2.87	1.42	1.33
13	A	802	CLA	C1C-C2C	2.87	1.50	1.44
13	B	814	CLA	MG-ND	-2.87	1.98	2.05
15	B	841	BCR	C12-C13	2.87	1.52	1.45
13	B	824	CLA	O2A-CGA	2.87	1.42	1.33
13	J	1103	CLA	C4A-NA	-2.87	1.33	1.39
13	B	834	CLA	C1C-C2C	2.87	1.50	1.44
15	F	1302	BCR	C19-C18	2.87	1.52	1.45
15	L	1005	BCR	C8-C9	2.87	1.52	1.45
15	L	1006	BCR	C8-C9	2.87	1.52	1.45
13	B	818	CLA	O2A-C1	-2.87	1.41	1.45
13	A	845	CLA	C4A-NA	-2.87	1.33	1.39
13	B	836	CLA	C4A-NA	-2.87	1.33	1.39
15	B	844	BCR	C26-C25	2.87	1.38	1.34
13	A	801	CLA	C1C-C2C	2.87	1.50	1.44
15	B	841	BCR	C19-C18	2.87	1.52	1.45
13	A	816	CLA	C1C-C2C	2.87	1.50	1.44
13	B	830	CLA	C4A-NA	-2.87	1.33	1.39
13	A	842	CLA	C1C-C2C	2.87	1.50	1.44
13	A	829	CLA	C1C-C2C	2.86	1.50	1.44
13	B	820	CLA	C1C-C2C	2.86	1.50	1.44
13	A	844	CLA	C4D-C3D	-2.86	1.38	1.41
15	B	847	BCR	C21-C22	2.86	1.39	1.35
13	J	1101	CLA	C4A-NA	-2.86	1.33	1.39
13	B	801	CLA	O2A-CGA	2.86	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	825	CLA	O2A-CGA	2.86	1.42	1.33
13	B	819	CLA	C4C-C3C	2.86	1.50	1.45
13	B	823	CLA	C1C-C2C	2.86	1.50	1.44
15	I	102	BCR	C8-C9	2.86	1.52	1.45
13	B	815	CLA	C4C-C3C	2.86	1.50	1.45
13	B	823	CLA	C4C-C3C	2.86	1.50	1.45
15	A	852	BCR	C8-C9	2.86	1.52	1.45
13	A	822	CLA	C4A-NA	-2.86	1.33	1.39
13	B	816	CLA	C1C-C2C	2.86	1.50	1.44
13	A	816	CLA	C4A-NA	-2.85	1.33	1.39
15	M	1203	BCR	C14-C13	2.85	1.39	1.35
13	A	826	CLA	C4A-NA	-2.85	1.33	1.39
15	B	849	BCR	C8-C9	2.85	1.52	1.45
13	A	805	CLA	MG-ND	-2.85	1.98	2.05
15	A	847	BCR	C19-C18	2.85	1.52	1.45
15	A	851	BCR	C26-C25	2.85	1.38	1.34
15	B	842	BCR	C12-C13	2.85	1.52	1.45
15	I	102	BCR	C26-C25	2.85	1.38	1.34
13	A	824	CLA	C4A-NA	-2.85	1.33	1.39
15	A	849	BCR	C8-C9	2.85	1.52	1.45
13	B	804	CLA	C4A-NA	-2.85	1.33	1.39
13	B	812	CLA	C1C-C2C	2.84	1.50	1.44
13	B	824	CLA	C4C-C3C	2.84	1.50	1.45
13	B	822	CLA	C4A-NA	-2.84	1.33	1.39
13	B	804	CLA	O2A-CGA	2.84	1.42	1.33
13	B	818	CLA	C4A-NA	-2.85	1.33	1.39
13	A	827	CLA	O2A-CGA	2.84	1.42	1.33
13	A	835	CLA	C1C-C2C	2.84	1.50	1.44
13	M	1202	CLA	C4C-C3C	2.84	1.50	1.45
13	A	808	CLA	O2D-CED	-2.84	1.38	1.45
13	B	824	CLA	C4A-NA	-2.84	1.33	1.39
13	B	802	CLA	O2A-CGA	2.84	1.42	1.33
13	B	812	CLA	C4A-NA	-2.84	1.33	1.39
13	A	815	CLA	C4C-C3C	2.83	1.50	1.45
15	F	1302	BCR	C12-C13	2.83	1.52	1.45
13	A	838	CLA	C4A-NA	-2.83	1.33	1.39
13	B	829	CLA	C1-C2	2.83	1.54	1.49
13	B	809	CLA	C1C-C2C	2.83	1.50	1.44
13	A	804	CLA	C4A-NA	-2.83	1.33	1.39
13	L	1002	CLA	C4A-NA	-2.83	1.33	1.39
13	B	832	CLA	C4A-NA	-2.83	1.33	1.39
13	B	818	CLA	O2D-CED	-2.83	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	831	CLA	O2D-CED	-2.83	1.38	1.45
13	B	827	CLA	C4A-NA	-2.83	1.33	1.39
13	A	831	CLA	C4A-NA	-2.83	1.33	1.39
13	A	812	CLA	C1C-C2C	2.83	1.50	1.44
13	B	815	CLA	O2D-CED	-2.83	1.38	1.45
15	B	846	BCR	C12-C13	2.83	1.52	1.45
15	B	841	BCR	C21-C22	2.83	1.39	1.35
13	B	801	CLA	C4C-C3C	2.83	1.50	1.45
13	B	830	CLA	MG-ND	-2.83	1.98	2.05
15	B	850	BCR	C26-C25	2.82	1.38	1.34
13	A	828	CLA	C4A-NA	-2.82	1.33	1.39
15	J	1104	BCR	C14-C13	2.82	1.39	1.35
13	A	824	CLA	C1C-C2C	2.82	1.50	1.44
13	B	829	CLA	C1C-C2C	2.82	1.50	1.44
15	B	841	BCR	C14-C13	2.82	1.39	1.35
13	A	803	CLA	C4A-NA	-2.82	1.33	1.39
13	A	855	CLA	C1C-C2C	2.82	1.50	1.44
13	A	841	CLA	C4A-NA	-2.82	1.33	1.39
13	A	841	CLA	O2A-CGA	2.82	1.42	1.33
13	X	102	CLA	C4A-NA	-2.82	1.33	1.39
13	B	834	CLA	C4C-C3C	2.82	1.50	1.45
15	A	849	BCR	C5-C6	2.82	1.38	1.34
13	B	806	CLA	C4A-NA	-2.82	1.33	1.39
13	A	855	CLA	C4C-C3C	2.82	1.50	1.45
13	B	839	CLA	C1C-C2C	2.81	1.50	1.44
13	L	1004	CLA	C1C-C2C	2.82	1.50	1.44
13	B	815	CLA	C4A-NA	-2.82	1.33	1.39
15	B	843	BCR	C26-C25	2.81	1.38	1.34
13	A	822	CLA	O2A-CGA	2.81	1.42	1.33
13	B	815	CLA	C1C-C2C	2.81	1.50	1.44
13	B	812	CLA	C4C-C3C	2.81	1.50	1.45
13	A	843	CLA	C4A-NA	-2.81	1.33	1.39
13	A	835	CLA	C4C-C3C	2.81	1.50	1.45
13	B	804	CLA	C1C-C2C	2.81	1.50	1.44
15	B	849	BCR	C19-C18	2.81	1.52	1.45
13	B	817	CLA	C4A-NA	-2.81	1.33	1.39
15	J	1104	BCR	C26-C25	2.81	1.38	1.34
13	A	832	CLA	C4A-NA	-2.81	1.33	1.39
13	B	831	CLA	O2A-CGA	2.81	1.42	1.33
13	A	842	CLA	C4A-NA	-2.81	1.33	1.39
13	A	822	CLA	C1C-C2C	2.81	1.50	1.44
13	B	808	CLA	C4A-NA	-2.81	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	805	CLA	C4A-NA	-2.81	1.33	1.39
13	A	839	CLA	C4C-C3C	2.81	1.50	1.45
15	L	1005	BCR	C21-C22	2.81	1.39	1.35
13	B	822	CLA	C4C-C3C	2.81	1.50	1.45
13	A	827	CLA	C4A-NA	-2.80	1.33	1.39
13	B	809	CLA	C4A-NA	-2.80	1.33	1.39
15	J	1105	BCR	C26-C25	2.80	1.38	1.34
13	L	1004	CLA	C4A-NA	-2.80	1.33	1.39
15	J	1104	BCR	C12-C13	2.80	1.52	1.45
13	B	822	CLA	O2A-CGA	2.80	1.42	1.33
15	B	847	BCR	C12-C13	2.80	1.52	1.45
13	A	825	CLA	C4A-NA	-2.80	1.33	1.39
13	B	808	CLA	O2A-CGA	2.80	1.42	1.33
13	B	808	CLA	C4C-C3C	2.80	1.50	1.45
13	B	805	CLA	C1C-C2C	2.80	1.50	1.44
13	A	841	CLA	C1C-C2C	2.80	1.50	1.44
13	B	818	CLA	C4C-C3C	2.80	1.50	1.45
13	A	830	CLA	O2A-CGA	2.80	1.42	1.33
13	B	817	CLA	C4C-C3C	2.79	1.50	1.45
13	B	811	CLA	C4A-NA	-2.79	1.33	1.39
15	F	1302	BCR	C21-C22	2.79	1.39	1.35
13	A	811	CLA	O2A-CGA	2.79	1.42	1.33
13	A	833	CLA	C4C-C3C	2.79	1.50	1.45
13	B	837	CLA	C4C-C3C	2.79	1.50	1.45
13	A	801	CLA	O2A-CGA	2.79	1.42	1.33
13	A	816	CLA	C4C-C3C	2.79	1.50	1.45
13	A	818	CLA	C4A-NA	-2.79	1.33	1.39
13	B	821	CLA	O2D-CED	-2.79	1.38	1.45
13	B	803	CLA	C1C-C2C	2.79	1.50	1.44
13	A	832	CLA	C4C-C3C	2.78	1.50	1.45
13	A	804	CLA	O2A-CGA	2.78	1.42	1.33
13	I	101	CLA	C4A-NA	-2.78	1.33	1.39
13	X	102	CLA	C1C-C2C	2.78	1.50	1.44
15	J	1105	BCR	C14-C13	2.78	1.39	1.35
13	B	838	CLA	C4A-NA	-2.78	1.33	1.39
13	A	803	CLA	O2D-CED	-2.78	1.38	1.45
13	A	817	CLA	C4A-NA	-2.78	1.33	1.39
13	A	805	CLA	C4C-C3C	2.78	1.50	1.45
13	B	833	CLA	C4A-NA	-2.77	1.33	1.39
13	A	821	CLA	C4C-C3C	2.78	1.50	1.45
13	B	822	CLA	C1C-C2C	2.78	1.50	1.44
13	J	1102	CLA	C4A-NA	-2.77	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	821	CLA	C1C-C2C	2.77	1.50	1.44
13	A	840	CLA	C4A-NA	-2.77	1.33	1.39
13	A	803	CLA	C4C-C3C	2.77	1.50	1.45
13	B	802	CLA	C4A-NA	-2.77	1.33	1.39
13	B	836	CLA	C4D-C3D	-2.77	1.38	1.41
13	A	820	CLA	C4C-C3C	2.77	1.50	1.45
13	A	808	CLA	C4A-NA	-2.77	1.33	1.39
13	L	1002	CLA	C4C-C3C	2.77	1.50	1.45
15	B	849	BCR	C5-C6	2.77	1.38	1.34
13	J	1101	CLA	O2A-CGA	2.77	1.42	1.33
13	A	815	CLA	C4A-NA	-2.77	1.33	1.39
15	B	843	BCR	C21-C22	2.77	1.39	1.35
13	A	829	CLA	O2A-CGA	2.77	1.41	1.33
13	B	809	CLA	C4C-C3C	2.77	1.50	1.45
13	A	839	CLA	C4A-NA	-2.77	1.33	1.39
13	A	812	CLA	C4A-NA	-2.77	1.33	1.39
13	A	834	CLA	O2A-CGA	2.77	1.41	1.33
13	B	828	CLA	C4A-NA	-2.77	1.33	1.39
13	A	836	CLA	C4C-C3C	2.77	1.50	1.45
13	B	814	CLA	C1C-C2C	2.76	1.50	1.44
13	B	813	CLA	C4C-C3C	2.76	1.50	1.45
15	J	1104	BCR	C5-C6	2.76	1.38	1.34
15	A	851	BCR	C12-C13	2.76	1.52	1.45
13	A	830	CLA	C4A-NA	-2.76	1.33	1.39
13	B	818	CLA	O2A-CGA	2.76	1.41	1.33
13	B	829	CLA	C4A-NA	-2.76	1.33	1.39
13	A	833	CLA	C4A-NA	-2.76	1.33	1.39
13	A	810	CLA	C1C-C2C	2.76	1.50	1.44
13	A	811	CLA	C4A-NA	-2.76	1.33	1.39
13	B	820	CLA	C4C-C3C	2.76	1.50	1.45
13	L	1004	CLA	O2A-CGA	2.76	1.41	1.33
13	A	821	CLA	O2A-CGA	2.76	1.41	1.33
13	B	822	CLA	C4D-C3D	-2.76	1.38	1.41
13	B	826	CLA	C4C-C3C	2.76	1.50	1.45
13	B	813	CLA	C1C-C2C	2.76	1.50	1.44
13	A	817	CLA	C4C-C3C	2.76	1.50	1.45
13	B	814	CLA	C4A-NA	-2.75	1.33	1.39
13	L	1003	CLA	C1C-C2C	2.75	1.50	1.44
13	A	816	CLA	O2A-CGA	2.75	1.41	1.33
13	A	830	CLA	MG-ND	-2.75	1.98	2.05
13	A	806	CLA	C4A-NA	-2.75	1.33	1.39
15	B	846	BCR	C5-C6	2.75	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	813	CLA	C4A-NA	-2.75	1.33	1.39
13	J	1102	CLA	C4C-C3C	2.75	1.50	1.45
13	A	840	CLA	C4C-C3C	2.75	1.50	1.45
13	A	818	CLA	C4C-C3C	2.75	1.50	1.45
13	B	828	CLA	C1C-C2C	2.75	1.50	1.44
13	A	804	CLA	O2D-CED	-2.75	1.38	1.45
13	B	812	CLA	C4D-C3D	-2.75	1.38	1.41
13	A	802	CLA	C4D-C3D	-2.75	1.38	1.41
13	A	833	CLA	C1C-C2C	2.75	1.50	1.44
13	A	805	CLA	O2A-CGA	2.74	1.41	1.33
13	B	839	CLA	O2A-CGA	2.74	1.41	1.33
13	B	810	CLA	C4C-C3C	2.75	1.50	1.45
13	B	830	CLA	C4B-NB	2.74	1.38	1.34
13	B	810	CLA	C1C-C2C	2.74	1.50	1.44
13	A	817	CLA	O2A-CGA	2.74	1.41	1.33
13	B	819	CLA	C1C-C2C	2.74	1.50	1.44
13	A	834	CLA	C4A-NA	-2.74	1.33	1.39
13	A	820	CLA	O2A-CGA	2.74	1.41	1.33
15	M	1203	BCR	C12-C13	2.74	1.52	1.45
13	A	839	CLA	O2A-CGA	2.74	1.41	1.33
13	B	831	CLA	C4C-C3C	2.74	1.50	1.45
13	A	842	CLA	C4C-C3C	2.74	1.50	1.45
13	A	839	CLA	C4D-C3D	-2.74	1.38	1.41
15	M	1203	BCR	C8-C9	2.74	1.52	1.45
13	B	825	CLA	C4C-C3C	2.74	1.50	1.45
13	A	810	CLA	C4A-NA	-2.74	1.33	1.39
15	A	847	BCR	C5-C6	2.74	1.38	1.34
13	B	831	CLA	C1C-C2C	2.74	1.50	1.44
13	A	814	CLA	C4C-C3C	2.74	1.50	1.45
13	A	826	CLA	C4C-C3C	2.74	1.50	1.45
13	A	803	CLA	O2A-CGA	2.74	1.41	1.33
13	B	827	CLA	O2A-CGA	2.73	1.41	1.33
13	L	1003	CLA	C4C-C3C	2.73	1.50	1.45
15	A	852	BCR	C12-C13	2.73	1.52	1.45
15	A	851	BCR	C14-C13	2.73	1.39	1.35
13	B	823	CLA	C4A-NA	-2.73	1.33	1.39
13	A	824	CLA	O2A-CGA	2.73	1.41	1.33
13	A	814	CLA	C4A-NA	-2.73	1.33	1.39
13	J	1101	CLA	C4C-C3C	2.73	1.50	1.45
13	B	838	CLA	C4C-C3C	2.73	1.50	1.45
13	A	812	CLA	C4C-C3C	2.73	1.50	1.45
13	F	1301	CLA	C4A-NA	-2.72	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	805	CLA	C4A-NA	-2.72	1.33	1.39
13	A	804	CLA	C4C-C3C	2.72	1.50	1.45
13	A	815	CLA	C1C-C2C	2.72	1.50	1.44
13	A	801	CLA	C4C-C3C	2.72	1.50	1.45
13	A	820	CLA	C1C-C2C	2.72	1.50	1.44
13	B	819	CLA	C4A-NA	-2.72	1.33	1.39
13	A	834	CLA	C1C-C2C	2.72	1.50	1.44
13	A	831	CLA	C4C-C3C	2.72	1.50	1.45
13	B	803	CLA	C4C-C3C	2.71	1.50	1.45
13	B	831	CLA	C4A-NA	-2.71	1.33	1.39
13	A	813	CLA	O2A-CGA	2.71	1.41	1.33
13	A	837	CLA	C4C-C3C	2.71	1.50	1.45
13	B	826	CLA	O2A-CGA	2.71	1.41	1.33
13	M	1201	CLA	C4C-C3C	2.71	1.50	1.45
18	B	848	LMG	O8-C28	2.71	1.41	1.33
13	I	101	CLA	O2A-CGA	2.71	1.41	1.33
13	A	836	CLA	C4A-NA	-2.71	1.33	1.39
15	I	102	BCR	C19-C18	2.71	1.51	1.45
13	B	803	CLA	O2A-CGA	2.71	1.41	1.33
15	A	849	BCR	C19-C18	2.71	1.51	1.45
13	A	842	CLA	O2A-CGA	2.71	1.41	1.33
13	A	827	CLA	C1C-C2C	2.71	1.50	1.44
13	B	820	CLA	C4A-NA	-2.71	1.33	1.39
13	A	833	CLA	O2A-CGA	2.71	1.41	1.33
13	B	837	CLA	O2A-CGA	2.71	1.41	1.33
13	B	838	CLA	O2A-CGA	2.71	1.41	1.33
13	B	830	CLA	O2A-CGA	2.71	1.41	1.33
13	B	835	CLA	C4A-NA	-2.71	1.33	1.39
13	A	837	CLA	C1A-NA	2.71	1.38	1.32
13	B	830	CLA	C4D-C3D	-2.71	1.38	1.41
13	A	835	CLA	O2A-CGA	2.70	1.41	1.33
13	B	836	CLA	O2A-CGA	2.70	1.41	1.33
13	A	809	CLA	O2A-CGA	2.70	1.41	1.33
13	B	835	CLA	C4C-C3C	2.70	1.50	1.45
13	A	828	CLA	C4C-C3C	2.70	1.50	1.45
13	F	1301	CLA	C4C-C3C	2.70	1.50	1.45
13	A	826	CLA	O2D-CED	-2.70	1.38	1.45
13	A	810	CLA	C4C-C3C	2.70	1.50	1.45
13	A	837	CLA	C4A-NA	-2.70	1.33	1.39
15	L	1006	BCR	C12-C13	2.70	1.51	1.45
13	A	825	CLA	C4C-C3C	2.70	1.50	1.45
13	B	828	CLA	C4C-C3C	2.70	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	806	CLA	O2D-CED	-2.69	1.38	1.45
13	B	829	CLA	O2A-CGA	2.69	1.41	1.33
13	A	831	CLA	C4D-C3D	-2.69	1.38	1.41
13	B	836	CLA	C4C-C3C	2.69	1.50	1.45
13	B	835	CLA	C1C-C2C	2.69	1.50	1.44
15	I	102	BCR	C14-C13	2.69	1.39	1.35
13	A	809	CLA	C4A-NA	-2.69	1.33	1.39
13	A	812	CLA	O2A-CGA	2.69	1.41	1.33
13	B	834	CLA	C4A-NA	-2.68	1.33	1.39
13	B	833	CLA	C4C-C3C	2.68	1.50	1.45
15	B	845	BCR	C5-C6	2.68	1.38	1.34
13	B	829	CLA	C4C-C3C	2.68	1.50	1.45
13	A	845	CLA	C1C-C2C	2.68	1.50	1.44
13	A	811	CLA	C4C-C3C	2.68	1.50	1.45
13	B	823	CLA	O2D-CED	-2.68	1.38	1.45
13	A	838	CLA	C4D-C3D	-2.68	1.38	1.41
13	B	813	CLA	C4D-C3D	-2.68	1.38	1.41
13	B	827	CLA	O2D-CED	-2.67	1.38	1.45
13	B	823	CLA	C1A-NA	2.67	1.38	1.32
13	A	828	CLA	O2A-CGA	2.67	1.41	1.33
13	B	826	CLA	C1C-C2C	2.67	1.50	1.44
15	A	850	BCR	C10-C9	2.67	1.39	1.35
13	B	817	CLA	C4D-C3D	-2.67	1.38	1.41
13	B	823	CLA	C4D-C3D	-2.67	1.38	1.41
13	A	819	CLA	C4D-C3D	-2.67	1.38	1.41
13	J	1103	CLA	C4D-C3D	-2.67	1.38	1.41
13	L	1002	CLA	O2A-CGA	2.67	1.41	1.33
13	B	815	CLA	C4D-C3D	-2.67	1.38	1.41
15	A	848	BCR	C5-C6	2.67	1.38	1.34
13	B	817	CLA	C1C-C2C	2.67	1.50	1.44
13	A	821	CLA	C4D-C3D	-2.67	1.38	1.41
13	M	1202	CLA	C4A-NA	-2.66	1.33	1.39
13	B	832	CLA	C4C-C3C	2.66	1.49	1.45
13	A	819	CLA	C1C-C2C	2.66	1.50	1.44
13	A	838	CLA	C4C-C3C	2.66	1.49	1.45
13	B	812	CLA	O2A-CGA	2.66	1.41	1.33
13	B	830	CLA	C4C-C3C	2.66	1.49	1.45
13	A	843	CLA	C4C-C3C	2.65	1.49	1.45
13	B	806	CLA	O2D-CED	-2.65	1.38	1.45
13	A	830	CLA	C4C-C3C	2.65	1.49	1.45
13	B	825	CLA	O2D-CED	-2.65	1.38	1.45
13	A	842	CLA	O2D-CED	-2.65	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	840	CLA	O2A-CGA	2.65	1.41	1.33
15	B	850	BCR	C5-C6	2.65	1.38	1.34
13	X	102	CLA	C4C-C3C	2.65	1.49	1.45
13	B	807	CLA	C4C-C3C	2.65	1.49	1.45
13	A	806	CLA	O2A-CGA	2.64	1.41	1.33
15	B	845	BCR	C12-C13	2.64	1.51	1.45
15	A	849	BCR	C21-C22	2.64	1.39	1.35
13	B	805	CLA	O2D-CED	-2.64	1.38	1.45
13	B	807	CLA	C4B-NB	2.64	1.37	1.34
13	B	825	CLA	O2A-CGA	2.63	1.41	1.33
13	M	1201	CLA	C4D-C3D	-2.63	1.38	1.41
15	A	851	BCR	C5-C6	2.63	1.38	1.34
13	B	816	CLA	C4C-C3C	2.63	1.49	1.45
13	A	818	CLA	C1C-C2C	2.63	1.50	1.44
15	L	1006	BCR	C10-C9	2.63	1.39	1.35
13	B	838	CLA	O2D-CED	-2.63	1.38	1.45
13	B	816	CLA	C4D-C3D	-2.63	1.38	1.41
15	F	1302	BCR	C5-C6	2.63	1.38	1.34
13	A	807	CLA	C3D-CAD	-2.63	1.42	1.47
13	B	804	CLA	C4C-C3C	2.63	1.49	1.45
13	B	832	CLA	O2D-CED	-2.62	1.38	1.45
13	A	845	CLA	O2A-CGA	2.62	1.41	1.33
13	B	839	CLA	C4D-C3D	-2.62	1.38	1.41
13	A	834	CLA	O2D-CED	-2.62	1.38	1.45
13	B	805	CLA	O2A-CGA	2.62	1.41	1.33
13	A	805	CLA	C3B-CAB	2.62	1.51	1.49
13	B	821	CLA	C4C-C3C	2.62	1.49	1.45
13	M	1202	CLA	C1A-NA	2.62	1.38	1.32
13	B	802	CLA	C4C-C3C	2.62	1.49	1.45
13	B	830	CLA	C3B-CAB	2.62	1.51	1.49
13	A	827	CLA	O2D-CED	-2.61	1.38	1.45
13	A	816	CLA	O2D-CED	-2.61	1.38	1.45
13	B	806	CLA	C4C-C3C	2.61	1.49	1.45
13	A	823	CLA	O2D-CED	-2.61	1.38	1.45
15	L	1005	BCR	C14-C13	2.61	1.39	1.35
13	A	822	CLA	O2D-CED	-2.61	1.38	1.45
13	B	817	CLA	O2A-CGA	2.60	1.41	1.33
13	A	823	CLA	O2A-CGA	2.60	1.41	1.33
13	B	806	CLA	C4D-C3D	-2.60	1.38	1.41
15	B	849	BCR	C12-C13	2.60	1.51	1.45
13	A	834	CLA	C4D-C3D	-2.60	1.38	1.41
15	I	102	BCR	C21-C22	2.60	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	829	CLA	O2D-CED	-2.60	1.38	1.45
13	F	1301	CLA	C1A-NA	2.60	1.38	1.32
13	B	814	CLA	C4C-C3C	2.60	1.49	1.45
13	B	825	CLA	C4D-C3D	-2.59	1.38	1.41
13	A	834	CLA	C4C-C3C	2.59	1.49	1.45
13	B	820	CLA	O2D-CED	-2.60	1.38	1.45
13	B	816	CLA	O2A-CGA	2.59	1.41	1.33
15	B	842	BCR	C5-C6	2.59	1.38	1.34
13	A	822	CLA	C4C-C3C	2.59	1.49	1.45
13	A	831	CLA	O2A-CGA	2.59	1.41	1.33
15	A	850	BCR	C5-C6	2.58	1.38	1.34
18	B	848	LMG	C4-C5	2.58	1.58	1.53
13	B	810	CLA	O2D-CED	-2.58	1.38	1.45
13	A	809	CLA	C4C-C3C	2.59	1.49	1.45
15	B	842	BCR	C10-C9	2.58	1.39	1.35
13	L	1004	CLA	O2D-CED	-2.58	1.38	1.45
13	A	805	CLA	C1A-NA	2.58	1.37	1.32
15	J	1105	BCR	C5-C6	2.58	1.38	1.34
13	A	833	CLA	O2D-CED	-2.58	1.38	1.45
13	A	819	CLA	C4C-C3C	2.58	1.49	1.45
13	B	806	CLA	O2A-CGA	2.58	1.41	1.33
13	A	826	CLA	C4D-C3D	-2.58	1.38	1.41
13	B	816	CLA	O2D-CED	-2.58	1.38	1.45
15	B	845	BCR	C14-C13	2.58	1.39	1.35
13	L	1002	CLA	O2D-CED	-2.58	1.38	1.45
13	I	101	CLA	O2D-CED	-2.58	1.38	1.45
13	B	805	CLA	C4D-C3D	-2.58	1.38	1.41
13	B	836	CLA	O2D-CED	-2.57	1.38	1.45
13	A	838	CLA	O2D-CED	-2.57	1.38	1.45
13	A	823	CLA	C4C-C3C	2.57	1.49	1.45
13	B	807	CLA	O2A-CGA	2.57	1.41	1.33
13	A	836	CLA	O2D-CED	-2.57	1.38	1.45
13	A	817	CLA	O2D-CED	-2.57	1.38	1.45
15	J	1104	BCR	C10-C9	2.57	1.39	1.35
15	B	850	BCR	C14-C13	2.57	1.39	1.35
13	A	838	CLA	O2A-CGA	2.57	1.41	1.33
13	I	101	CLA	C4C-C3C	2.57	1.49	1.45
13	A	835	CLA	O2D-CED	-2.57	1.38	1.45
13	A	841	CLA	O2D-CED	-2.57	1.38	1.45
15	A	849	BCR	C12-C13	2.57	1.51	1.45
15	B	841	BCR	C5-C6	2.57	1.38	1.34
13	A	843	CLA	O2D-CED	-2.57	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	802	CLA	O2D-CED	-2.57	1.38	1.45
13	A	819	CLA	O2A-CGA	2.57	1.41	1.33
13	A	830	CLA	O2D-CED	-2.57	1.38	1.45
13	A	808	CLA	C4C-C3C	2.56	1.49	1.45
13	A	817	CLA	O2D-CGD	2.56	1.39	1.33
13	L	1003	CLA	O2D-CED	-2.56	1.38	1.45
13	A	808	CLA	C1A-NA	2.56	1.37	1.32
15	B	849	BCR	C14-C13	2.56	1.39	1.35
13	B	814	CLA	O2A-CGA	2.56	1.41	1.33
13	B	830	CLA	O2D-CED	-2.56	1.38	1.45
13	A	809	CLA	O2D-CED	-2.56	1.38	1.45
15	B	842	BCR	C24-C23	2.55	1.40	1.32
13	A	833	CLA	C4B-NB	2.55	1.37	1.34
13	A	825	CLA	O2D-CED	-2.55	1.38	1.45
13	B	803	CLA	O2D-CED	-2.55	1.39	1.45
13	B	815	CLA	O2A-CGA	2.55	1.41	1.33
13	A	807	CLA	O2A-CGA	2.55	1.41	1.33
13	B	804	CLA	O2D-CED	-2.55	1.39	1.45
13	A	842	CLA	C4D-C3D	-2.55	1.38	1.41
13	A	841	CLA	C4D-C3D	-2.54	1.38	1.41
13	A	817	CLA	C4D-C3D	-2.54	1.38	1.41
13	A	801	CLA	O2D-CED	-2.54	1.39	1.45
13	B	833	CLA	C4D-C3D	-2.54	1.38	1.41
13	F	1301	CLA	O2D-CED	-2.54	1.39	1.45
13	A	845	CLA	O2D-CED	-2.54	1.39	1.45
13	A	815	CLA	O2D-CED	-2.54	1.39	1.45
13	B	821	CLA	O2D-CGD	2.54	1.39	1.33
13	J	1101	CLA	O2D-CED	-2.54	1.39	1.45
15	A	852	BCR	C5-C6	2.54	1.38	1.34
13	A	829	CLA	O2D-CED	-2.54	1.39	1.45
13	A	805	CLA	O2D-CED	-2.53	1.39	1.45
13	A	855	CLA	O2D-CED	-2.53	1.39	1.45
13	A	802	CLA	O2D-CED	-2.53	1.39	1.45
13	B	811	CLA	O2D-CED	-2.53	1.39	1.45
13	B	837	CLA	O2D-CED	-2.53	1.39	1.45
13	A	820	CLA	O2D-CED	-2.53	1.39	1.45
13	A	807	CLA	C4C-C3C	2.53	1.49	1.45
13	B	810	CLA	C4D-C3D	-2.53	1.38	1.41
15	L	1005	BCR	C5-C6	2.53	1.38	1.34
13	A	824	CLA	O2D-CED	-2.53	1.39	1.45
13	A	835	CLA	C4D-C3D	-2.53	1.38	1.41
13	A	804	CLA	C1A-NA	2.53	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	810	CLA	O2D-CGD	2.53	1.39	1.33
13	A	843	CLA	O2A-CGA	2.52	1.41	1.33
15	A	847	BCR	C10-C9	2.52	1.39	1.35
13	A	811	CLA	O2D-CED	-2.52	1.39	1.45
13	A	821	CLA	O2D-CED	-2.52	1.39	1.45
15	A	848	BCR	C10-C9	2.52	1.39	1.35
13	A	806	CLA	C4D-C3D	-2.52	1.38	1.41
15	A	850	BCR	C24-C23	2.52	1.40	1.32
13	A	813	CLA	O2D-CED	-2.52	1.39	1.45
13	B	838	CLA	C4D-C3D	-2.52	1.38	1.41
13	A	833	CLA	O2D-CGD	2.52	1.39	1.33
13	B	822	CLA	O2D-CED	-2.52	1.39	1.45
13	B	814	CLA	O2D-CED	-2.52	1.39	1.45
13	A	807	CLA	C4A-NA	-2.52	1.33	1.39
13	B	839	CLA	O2D-CED	-2.52	1.39	1.45
13	A	855	CLA	C4D-C3D	-2.52	1.38	1.41
13	A	826	CLA	C1A-NA	2.52	1.37	1.32
13	M	1201	CLA	O2D-CED	-2.51	1.39	1.45
13	A	810	CLA	O2D-CED	-2.51	1.39	1.45
15	B	841	BCR	C10-C9	2.51	1.39	1.35
13	A	840	CLA	O2D-CED	-2.51	1.39	1.45
13	A	840	CLA	C4D-C3D	-2.51	1.38	1.41
13	J	1102	CLA	C4B-NB	2.51	1.37	1.34
13	A	818	CLA	C4D-C3D	-2.51	1.38	1.41
15	A	852	BCR	C24-C23	2.51	1.40	1.32
13	B	808	CLA	O2D-CED	-2.51	1.39	1.45
13	A	807	CLA	C4D-C3D	-2.50	1.38	1.41
13	A	832	CLA	O2D-CED	-2.51	1.39	1.45
13	B	802	CLA	C3D-CAD	-2.50	1.42	1.47
13	B	834	CLA	O2D-CED	-2.50	1.39	1.45
13	B	819	CLA	C1A-NA	2.50	1.37	1.32
13	A	840	CLA	C4B-NB	2.50	1.37	1.34
13	B	801	CLA	O2D-CED	-2.50	1.39	1.45
13	F	1301	CLA	C4D-C3D	-2.50	1.38	1.41
13	A	804	CLA	C4D-C3D	-2.50	1.38	1.41
13	A	807	CLA	C1A-NA	2.50	1.37	1.32
13	B	820	CLA	C4D-C3D	-2.50	1.38	1.41
15	B	845	BCR	C24-C23	2.50	1.40	1.32
13	B	812	CLA	O2D-CED	-2.50	1.39	1.45
13	A	818	CLA	O2A-CGA	2.50	1.41	1.33
15	B	843	BCR	C5-C6	2.50	1.38	1.34
13	B	819	CLA	O2D-CED	-2.50	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	102	CLA	O2D-CED	-2.49	1.39	1.45
13	A	833	CLA	C4D-C3D	-2.49	1.38	1.41
13	A	823	CLA	C4D-C3D	-2.49	1.38	1.41
13	A	839	CLA	O2D-CED	-2.49	1.39	1.45
15	I	102	BCR	C12-C13	2.49	1.51	1.45
13	B	807	CLA	O2D-CED	-2.49	1.39	1.45
13	B	825	CLA	C1A-NA	2.49	1.37	1.32
13	B	828	CLA	O2D-CED	-2.49	1.39	1.45
13	A	818	CLA	O2D-CED	-2.49	1.39	1.45
13	B	809	CLA	O2D-CED	-2.48	1.39	1.45
13	B	829	CLA	O2D-CGD	2.48	1.39	1.33
13	A	812	CLA	O2D-CED	-2.48	1.39	1.45
13	B	834	CLA	C1A-NA	2.48	1.37	1.32
15	B	845	BCR	C40-C30	-2.48	1.48	1.53
13	B	837	CLA	C4D-C3D	-2.48	1.38	1.41
13	B	833	CLA	O2D-CED	-2.48	1.39	1.45
13	A	828	CLA	C1A-NA	2.48	1.37	1.32
13	B	821	CLA	C4B-NB	2.47	1.37	1.34
13	A	823	CLA	C1A-NA	2.47	1.37	1.32
13	A	818	CLA	C1A-NA	2.47	1.37	1.32
13	B	824	CLA	O2D-CED	-2.47	1.39	1.45
13	A	841	CLA	O2D-CGD	2.47	1.39	1.33
13	B	808	CLA	C1A-NA	2.47	1.37	1.32
13	A	828	CLA	O2D-CED	-2.47	1.39	1.45
13	A	819	CLA	O2D-CED	-2.47	1.39	1.45
13	A	816	CLA	O2D-CGD	2.47	1.39	1.33
13	I	101	CLA	O2D-CGD	2.47	1.39	1.33
13	B	820	CLA	C4B-NB	2.47	1.37	1.34
13	A	821	CLA	C4B-NB	2.47	1.37	1.34
15	B	845	BCR	C26-C25	2.47	1.38	1.34
13	J	1102	CLA	C4D-C3D	-2.46	1.38	1.41
15	I	102	BCR	C32-C1	-2.46	1.48	1.53
13	A	828	CLA	C4B-NB	2.46	1.37	1.34
13	A	828	CLA	O2D-CGD	2.46	1.39	1.33
13	A	828	CLA	C3B-CAB	2.46	1.51	1.49
13	A	811	CLA	C4D-C3D	-2.46	1.38	1.41
13	A	842	CLA	O2D-CGD	2.46	1.39	1.33
15	B	843	BCR	C32-C1	-2.46	1.48	1.53
15	J	1105	BCR	C10-C9	2.46	1.39	1.35
13	B	831	CLA	C1A-NA	2.45	1.37	1.32
13	M	1202	CLA	O2D-CED	-2.45	1.39	1.45
13	B	814	CLA	C1A-NA	2.45	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	1104	BCR	C24-C23	2.45	1.40	1.32
13	B	824	CLA	C4D-C3D	-2.45	1.38	1.41
13	B	820	CLA	O2D-CGD	2.45	1.39	1.33
15	B	846	BCR	C32-C1	-2.45	1.48	1.53
18	B	848	LMG	O6-C1	2.45	1.48	1.41
13	B	814	CLA	C4B-NB	2.45	1.37	1.34
13	A	801	CLA	C1A-NA	2.44	1.37	1.32
13	A	808	CLA	C3D-CAD	-2.44	1.42	1.47
13	L	1002	CLA	C4D-C3D	-2.44	1.38	1.41
15	B	850	BCR	C10-C9	2.44	1.39	1.35
13	A	842	CLA	C4B-NB	2.44	1.37	1.34
13	I	101	CLA	C4D-C3D	-2.44	1.38	1.41
13	B	830	CLA	O2D-CGD	2.44	1.39	1.33
13	M	1202	CLA	C4D-C3D	-2.44	1.38	1.41
13	J	1102	CLA	O2D-CED	-2.44	1.39	1.45
13	A	823	CLA	O2D-CGD	2.44	1.39	1.33
13	L	1004	CLA	C4B-NB	2.44	1.37	1.34
13	A	811	CLA	C1A-NA	2.43	1.37	1.32
13	A	809	CLA	O2D-CGD	2.43	1.39	1.33
13	J	1102	CLA	C1A-NA	2.43	1.37	1.32
15	L	1005	BCR	C32-C1	-2.43	1.48	1.53
13	B	809	CLA	C4D-C3D	-2.43	1.38	1.41
13	M	1202	CLA	C4B-NB	2.43	1.37	1.34
13	A	845	CLA	C4D-C3D	-2.43	1.38	1.41
15	J	1105	BCR	C32-C1	-2.43	1.48	1.53
13	B	813	CLA	O2D-CED	-2.43	1.39	1.45
13	A	807	CLA	O2D-CED	-2.43	1.39	1.45
13	B	824	CLA	C1A-NA	2.43	1.37	1.32
13	A	839	CLA	C1A-NA	2.43	1.37	1.32
15	A	852	BCR	C20-C19	2.42	1.41	1.34
13	A	835	CLA	O2D-CGD	2.42	1.39	1.33
15	B	847	BCR	C32-C1	-2.42	1.48	1.53
15	B	847	BCR	C5-C6	2.42	1.38	1.34
13	B	802	CLA	C4D-C3D	-2.42	1.38	1.41
13	B	834	CLA	C4D-C3D	-2.42	1.38	1.41
13	B	808	CLA	C4D-C3D	-2.42	1.38	1.41
13	A	823	CLA	C4B-NB	2.42	1.37	1.34
15	B	847	BCR	C24-C23	2.42	1.40	1.32
15	A	847	BCR	C24-C23	2.42	1.40	1.32
15	B	846	BCR	C10-C9	2.42	1.38	1.35
13	B	833	CLA	C4B-NB	2.42	1.37	1.34
13	B	809	CLA	C4B-NB	2.42	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	837	CLA	C4B-NB	2.41	1.37	1.34
15	B	850	BCR	C32-C1	-2.42	1.48	1.53
13	A	810	CLA	C1A-NA	2.41	1.37	1.32
13	A	820	CLA	O2D-CGD	2.41	1.39	1.33
15	A	849	BCR	C32-C1	-2.41	1.48	1.53
15	A	849	BCR	C14-C13	2.41	1.38	1.35
13	B	828	CLA	C1A-NA	2.41	1.37	1.32
15	B	844	BCR	C24-C23	2.41	1.40	1.32
13	B	827	CLA	C1A-NA	2.41	1.37	1.32
13	B	809	CLA	C1A-NA	2.41	1.37	1.32
13	B	817	CLA	O2D-CED	-2.41	1.39	1.45
13	X	102	CLA	C4D-C3D	-2.40	1.38	1.41
13	A	836	CLA	C4B-NB	2.40	1.37	1.34
13	A	817	CLA	C4B-NB	2.40	1.37	1.34
13	B	804	CLA	C1A-NA	2.40	1.37	1.32
15	A	851	BCR	C32-C1	-2.40	1.48	1.53
13	A	816	CLA	C4D-C3D	-2.40	1.38	1.41
15	B	846	BCR	C24-C23	2.39	1.40	1.32
15	B	842	BCR	C32-C1	-2.39	1.48	1.53
13	B	836	CLA	C4B-NB	2.39	1.37	1.34
15	B	847	BCR	C10-C9	2.39	1.38	1.35
13	M	1202	CLA	O2D-CGD	2.39	1.39	1.33
13	B	834	CLA	C4B-NB	2.39	1.37	1.34
13	L	1004	CLA	C4D-C3D	-2.39	1.38	1.41
13	B	832	CLA	C4D-C3D	-2.39	1.38	1.41
13	B	814	CLA	C4D-C3D	-2.39	1.38	1.41
13	A	814	CLA	C4D-C3D	-2.39	1.38	1.41
15	A	852	BCR	C10-C9	2.39	1.38	1.35
13	B	832	CLA	C4B-NB	2.38	1.37	1.34
13	J	1101	CLA	C1A-NA	2.38	1.37	1.32
13	A	830	CLA	C3B-CAB	2.38	1.51	1.49
15	J	1105	BCR	C24-C23	2.38	1.40	1.32
15	B	849	BCR	C32-C1	-2.38	1.48	1.53
13	B	820	CLA	C1A-NA	2.38	1.37	1.32
13	B	825	CLA	C4B-NB	2.38	1.37	1.34
13	A	803	CLA	C4D-C3D	-2.38	1.38	1.41
13	B	818	CLA	C4D-C3D	-2.38	1.38	1.41
15	J	1104	BCR	C32-C1	-2.37	1.48	1.53
13	B	835	CLA	C1A-NA	2.37	1.37	1.32
13	A	809	CLA	C4B-NB	2.37	1.37	1.34
13	A	830	CLA	C1A-NA	2.37	1.37	1.32
15	A	850	BCR	C32-C1	-2.37	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	815	CLA	C4B-NB	2.37	1.37	1.34
13	A	826	CLA	C4B-NB	2.37	1.37	1.34
15	B	841	BCR	C24-C23	2.37	1.39	1.32
15	L	1006	BCR	C24-C23	2.37	1.39	1.32
13	B	828	CLA	O2D-CGD	2.37	1.39	1.33
13	B	818	CLA	C1A-NA	2.37	1.37	1.32
13	A	828	CLA	C4D-C3D	-2.36	1.38	1.41
13	A	829	CLA	C4D-C3D	-2.36	1.38	1.41
15	L	1005	BCR	C10-C9	2.36	1.38	1.35
13	A	833	CLA	C1A-NA	2.36	1.37	1.32
13	L	1004	CLA	C1A-NA	2.36	1.37	1.32
13	B	815	CLA	C1A-NA	2.36	1.37	1.32
13	B	811	CLA	C1A-NA	2.36	1.37	1.32
15	A	848	BCR	C24-C23	2.36	1.39	1.32
15	M	1203	BCR	C32-C1	-2.36	1.48	1.53
13	B	803	CLA	C4D-C3D	-2.36	1.38	1.41
13	B	813	CLA	O2D-CGD	2.36	1.39	1.33
13	B	825	CLA	O2D-CGD	2.36	1.39	1.33
13	B	803	CLA	C1A-NA	2.36	1.37	1.32
13	A	808	CLA	C4D-C3D	-2.36	1.38	1.41
15	L	1006	BCR	C32-C1	-2.36	1.48	1.53
13	B	822	CLA	C1A-NA	2.36	1.37	1.32
13	F	1301	CLA	O2D-CGD	2.36	1.39	1.33
13	A	807	CLA	C4B-NB	2.36	1.37	1.34
13	B	805	CLA	C4B-NB	2.36	1.37	1.34
13	A	825	CLA	C1A-NA	2.36	1.37	1.32
13	A	818	CLA	O2D-CGD	2.36	1.39	1.33
15	A	848	BCR	C32-C1	-2.36	1.48	1.53
15	F	1302	BCR	C10-C9	2.35	1.38	1.35
15	L	1005	BCR	C24-C23	2.35	1.39	1.32
13	J	1102	CLA	O2D-CGD	2.35	1.39	1.33
13	B	816	CLA	O2D-CGD	2.35	1.39	1.33
13	A	827	CLA	C4C-C3C	2.35	1.49	1.45
13	B	822	CLA	C3B-CAB	2.35	1.51	1.49
13	B	834	CLA	C3B-CAB	2.35	1.51	1.49
15	B	850	BCR	C24-C23	2.35	1.39	1.32
13	B	801	CLA	O2D-CGD	2.35	1.39	1.33
15	A	847	BCR	C32-C1	-2.35	1.48	1.53
15	A	852	BCR	C32-C1	-2.35	1.48	1.53
13	B	805	CLA	O2D-CGD	2.35	1.39	1.33
13	A	836	CLA	C4D-C3D	-2.35	1.38	1.41
13	A	805	CLA	C4B-NB	2.34	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	812	CLA	O2D-CGD	2.34	1.39	1.33
13	B	827	CLA	C4D-C3D	-2.34	1.38	1.41
13	A	840	CLA	O2D-CGD	2.34	1.39	1.33
13	A	806	CLA	O2D-CGD	2.34	1.39	1.33
13	A	815	CLA	O2D-CGD	2.34	1.39	1.33
15	B	847	BCR	C40-C30	-2.34	1.48	1.53
15	A	851	BCR	C10-C9	2.34	1.38	1.35
13	B	829	CLA	C1A-NA	2.34	1.37	1.32
13	A	835	CLA	C4B-NB	2.34	1.37	1.34
13	B	833	CLA	C1A-NA	2.33	1.37	1.32
13	A	832	CLA	C5-C3	2.33	1.56	1.51
15	B	845	BCR	C32-C1	-2.33	1.48	1.53
13	A	845	CLA	C4B-NB	2.33	1.37	1.34
13	A	802	CLA	O2D-CGD	2.33	1.39	1.33
13	A	813	CLA	C4D-C3D	-2.33	1.38	1.41
13	L	1003	CLA	C4D-C3D	-2.33	1.38	1.41
13	A	817	CLA	C1A-NA	2.33	1.37	1.32
13	B	819	CLA	O2D-CGD	2.33	1.39	1.33
15	A	851	BCR	C24-C23	2.33	1.39	1.32
13	B	801	CLA	C1A-NA	2.33	1.37	1.32
13	B	804	CLA	C3B-CAB	2.33	1.51	1.49
13	B	824	CLA	C4B-NB	2.33	1.37	1.34
13	A	827	CLA	C1A-NA	2.33	1.37	1.32
13	B	813	CLA	C1A-NA	2.32	1.37	1.32
13	A	834	CLA	O2D-CGD	2.32	1.39	1.33
13	B	820	CLA	O2A-CGA	2.32	1.40	1.33
13	A	804	CLA	C4B-NB	2.32	1.37	1.34
15	M	1203	BCR	C24-C23	2.32	1.39	1.32
13	B	803	CLA	C4B-NB	2.32	1.37	1.34
13	A	813	CLA	C4B-NB	2.32	1.37	1.34
13	J	1101	CLA	C4D-C3D	-2.32	1.38	1.41
13	A	819	CLA	O2D-CGD	2.32	1.39	1.33
13	B	815	CLA	O2D-CGD	2.32	1.39	1.33
13	A	806	CLA	C1A-NA	2.32	1.37	1.32
15	A	849	BCR	C24-C23	2.32	1.39	1.32
13	B	828	CLA	C4D-C3D	-2.32	1.38	1.41
13	M	1201	CLA	C4B-NB	2.32	1.37	1.34
13	B	831	CLA	C4B-NB	2.32	1.37	1.34
15	B	841	BCR	C32-C1	-2.32	1.48	1.53
13	B	811	CLA	C4D-C3D	-2.32	1.38	1.41
13	A	812	CLA	C4D-C3D	-2.32	1.38	1.41
13	A	836	CLA	O2D-CGD	2.32	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	811	CLA	C5-C3	2.32	1.56	1.51
13	M	1201	CLA	C3D-CAD	-2.31	1.42	1.47
13	A	810	CLA	C4D-C3D	-2.31	1.38	1.41
15	F	1302	BCR	C32-C1	-2.31	1.48	1.53
13	B	823	CLA	O2D-CGD	2.31	1.39	1.33
13	A	807	CLA	CBD-CAD	-2.31	1.45	1.56
13	A	803	CLA	C4B-NB	2.31	1.37	1.34
13	A	825	CLA	C5-C3	2.31	1.56	1.51
13	A	809	CLA	C1A-NA	2.31	1.37	1.32
13	A	809	CLA	C4D-C3D	-2.31	1.38	1.41
13	A	815	CLA	C4D-C3D	-2.31	1.38	1.41
13	B	802	CLA	C1A-NA	2.31	1.37	1.32
13	A	841	CLA	C1A-NA	2.31	1.37	1.32
13	B	837	CLA	O2D-CGD	2.31	1.39	1.33
13	A	820	CLA	C1A-NA	2.31	1.37	1.32
13	A	838	CLA	O2D-CGD	2.31	1.39	1.33
13	M	1202	CLA	C3B-CAB	2.31	1.51	1.49
13	B	835	CLA	C4D-C3D	-2.31	1.38	1.41
13	A	855	CLA	O2D-CGD	2.31	1.39	1.33
15	B	849	BCR	C24-C23	2.31	1.39	1.32
13	A	831	CLA	C4B-NB	2.31	1.37	1.34
13	B	839	CLA	O2D-CGD	2.31	1.39	1.33
13	A	829	CLA	C4B-NB	2.31	1.37	1.34
13	A	803	CLA	C1A-NA	2.30	1.37	1.32
13	A	812	CLA	C4B-NB	2.31	1.37	1.34
13	A	834	CLA	C5-C3	2.30	1.56	1.51
13	A	843	CLA	O2D-CGD	2.30	1.39	1.33
13	A	810	CLA	C4B-NB	2.30	1.37	1.34
13	A	827	CLA	C4D-C3D	-2.30	1.38	1.41
13	B	804	CLA	O2D-CGD	2.30	1.39	1.33
13	A	802	CLA	C4B-NB	2.30	1.37	1.34
13	B	808	CLA	C4B-NB	2.30	1.37	1.34
13	B	830	CLA	C1A-NA	2.30	1.37	1.32
13	A	825	CLA	C4D-C3D	-2.30	1.38	1.41
13	A	832	CLA	C4D-C3D	-2.30	1.38	1.41
13	L	1002	CLA	C3B-CAB	2.30	1.51	1.49
13	A	826	CLA	O2D-CGD	2.29	1.39	1.33
13	B	832	CLA	O2D-CGD	2.29	1.39	1.33
13	A	845	CLA	O2D-CGD	2.29	1.39	1.33
13	B	821	CLA	C4D-C3D	-2.29	1.38	1.41
13	B	806	CLA	O2D-CGD	2.29	1.39	1.33
13	A	813	CLA	C1A-NA	2.29	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	824	CLA	C3B-CAB	2.29	1.51	1.49
13	A	824	CLA	C4D-C3D	-2.29	1.38	1.41
13	A	825	CLA	O2D-CGD	2.29	1.39	1.33
13	A	832	CLA	O2D-CGD	2.29	1.39	1.33
13	B	817	CLA	C3B-CAB	2.29	1.51	1.49
13	B	827	CLA	C4C-C3C	2.29	1.49	1.45
13	B	823	CLA	C4B-NB	2.29	1.37	1.34
13	B	818	CLA	O2D-CGD	2.28	1.39	1.33
18	B	848	LMG	C4-C3	2.28	1.58	1.52
13	B	812	CLA	CBD-CAD	-2.28	1.46	1.56
15	B	842	BCR	C40-C30	-2.28	1.48	1.53
13	B	801	CLA	C4D-C3D	-2.28	1.38	1.41
18	B	848	LMG	C3-C2	2.28	1.58	1.52
13	A	804	CLA	O2D-CGD	2.28	1.39	1.33
15	M	1203	BCR	C40-C30	-2.28	1.48	1.53
13	B	819	CLA	C4B-NB	2.28	1.37	1.34
18	B	848	LMG	O7-C8	-2.28	1.40	1.46
13	A	842	CLA	C3B-CAB	2.28	1.51	1.49
13	B	821	CLA	C3B-CAB	2.28	1.51	1.49
15	B	844	BCR	C20-C19	2.28	1.40	1.34
13	A	845	CLA	C1A-NA	2.27	1.37	1.32
13	A	810	CLA	O2D-CGD	2.27	1.39	1.33
13	X	102	CLA	C4B-NB	2.27	1.37	1.34
13	A	823	CLA	C3B-CAB	2.27	1.51	1.49
13	B	802	CLA	O2D-CGD	2.27	1.39	1.33
13	A	812	CLA	O2D-CGD	2.27	1.39	1.33
13	M	1201	CLA	O2D-CGD	2.27	1.39	1.33
13	B	824	CLA	O2D-CGD	2.27	1.39	1.33
15	B	845	BCR	C10-C9	2.27	1.38	1.35
13	L	1002	CLA	C4B-NB	2.27	1.37	1.34
15	F	1302	BCR	C24-C23	2.27	1.39	1.32
13	B	829	CLA	C4B-NB	2.27	1.37	1.34
13	A	804	CLA	C3D-CAD	-2.27	1.42	1.47
13	B	834	CLA	O2D-CGD	2.27	1.39	1.33
13	A	805	CLA	O2D-CGD	2.27	1.39	1.33
13	A	842	CLA	C5-C3	2.27	1.56	1.51
13	A	822	CLA	C4B-NB	2.26	1.37	1.34
15	B	843	BCR	C40-C30	-2.27	1.48	1.53
13	A	839	CLA	O2D-CGD	2.27	1.39	1.33
13	A	843	CLA	C1A-NA	2.26	1.37	1.32
13	A	832	CLA	C4B-NB	2.26	1.37	1.34
13	B	828	CLA	C3B-C2B	-2.26	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	819	CLA	C4D-C3D	-2.26	1.38	1.41
13	B	839	CLA	C4B-NB	2.26	1.37	1.34
13	B	801	CLA	C4B-NB	2.26	1.37	1.34
13	A	829	CLA	C5-C3	2.26	1.56	1.51
13	B	809	CLA	O2D-CGD	2.26	1.39	1.33
13	A	839	CLA	C4B-NB	2.26	1.37	1.34
15	B	844	BCR	C40-C30	-2.26	1.48	1.53
13	A	840	CLA	C1A-NA	2.26	1.37	1.32
13	A	829	CLA	C1A-NA	2.26	1.37	1.32
13	J	1101	CLA	O2D-CGD	2.25	1.39	1.33
15	A	850	BCR	C20-C19	2.25	1.40	1.34
15	I	102	BCR	C24-C23	2.25	1.39	1.32
13	B	817	CLA	O2D-CGD	2.25	1.39	1.33
13	A	834	CLA	C3B-C2B	-2.25	1.37	1.41
15	B	843	BCR	C10-C9	2.25	1.38	1.35
13	A	822	CLA	O2D-CGD	2.25	1.39	1.33
13	A	829	CLA	O2D-CGD	2.25	1.39	1.33
13	B	807	CLA	O2D-CGD	2.25	1.39	1.33
13	A	838	CLA	C5-C3	2.25	1.56	1.51
13	A	821	CLA	C1A-NA	2.25	1.37	1.32
13	B	805	CLA	C1A-NA	2.25	1.37	1.32
13	A	816	CLA	C1A-NA	2.25	1.37	1.32
13	B	811	CLA	O2D-CGD	2.25	1.39	1.33
13	A	811	CLA	C4B-NB	2.25	1.37	1.34
15	J	1105	BCR	C20-C19	2.25	1.40	1.34
15	I	102	BCR	C40-C30	-2.25	1.48	1.53
13	A	827	CLA	O2D-CGD	2.24	1.39	1.33
13	A	821	CLA	C3B-CAB	2.24	1.51	1.49
15	B	842	BCR	C8-C7	2.24	1.39	1.32
13	A	813	CLA	O2D-CGD	2.24	1.39	1.33
13	A	830	CLA	C5-C3	2.24	1.56	1.51
13	B	802	CLA	CBD-CAD	-2.24	1.46	1.56
13	A	837	CLA	C3D-CAD	-2.24	1.42	1.47
13	B	812	CLA	C1A-NA	2.24	1.37	1.32
13	A	803	CLA	O2D-CGD	2.24	1.39	1.33
13	A	818	CLA	C4B-NB	2.24	1.37	1.34
15	J	1105	BCR	C40-C30	-2.24	1.48	1.53
13	X	102	CLA	C1A-NA	2.24	1.37	1.32
13	X	102	CLA	O2D-CGD	2.24	1.39	1.33
13	B	828	CLA	C4B-NB	2.24	1.37	1.34
13	B	836	CLA	O2D-CGD	2.24	1.39	1.33
15	B	843	BCR	C24-C23	2.23	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	826	CLA	C4B-NB	2.24	1.37	1.34
13	B	832	CLA	C1A-NA	2.23	1.37	1.32
13	A	815	CLA	C1A-NA	2.23	1.37	1.32
15	I	102	BCR	C5-C6	2.23	1.37	1.34
15	L	1005	BCR	C40-C30	-2.23	1.48	1.53
13	B	809	CLA	C3B-CAB	2.23	1.51	1.49
13	B	832	CLA	C3B-CAB	2.23	1.51	1.49
13	A	806	CLA	C4B-NB	2.23	1.37	1.34
13	B	812	CLA	C3D-CAD	-2.23	1.42	1.47
13	A	855	CLA	C1A-NA	2.23	1.37	1.32
13	A	841	CLA	C4B-NB	2.23	1.37	1.34
13	L	1004	CLA	O2D-CGD	2.23	1.39	1.33
13	A	821	CLA	O2D-CGD	2.23	1.39	1.33
13	B	830	CLA	C5-C3	2.23	1.56	1.51
13	B	804	CLA	C4D-C3D	-2.23	1.38	1.41
13	A	801	CLA	C4D-C3D	-2.23	1.38	1.41
13	B	807	CLA	C3D-CAD	-2.23	1.42	1.47
13	B	823	CLA	C3D-CAD	-2.23	1.42	1.47
13	B	806	CLA	C4B-NB	2.23	1.37	1.34
13	A	830	CLA	O2D-CGD	2.23	1.39	1.33
13	I	101	CLA	C3D-CAD	-2.22	1.42	1.47
13	A	825	CLA	C4B-NB	2.22	1.37	1.34
13	B	835	CLA	C5-C3	2.22	1.56	1.51
13	B	807	CLA	CBD-CAD	-2.22	1.46	1.56
13	A	821	CLA	C5-C3	2.22	1.56	1.51
13	A	805	CLA	C5-C3	2.22	1.56	1.51
15	B	850	BCR	C8-C7	2.22	1.39	1.32
13	B	833	CLA	O2D-CGD	2.22	1.39	1.33
13	A	804	CLA	C3B-CAB	2.22	1.51	1.49
13	B	826	CLA	C4D-C3D	-2.22	1.38	1.41
13	B	838	CLA	C1A-NA	2.22	1.37	1.32
13	B	814	CLA	O2D-CGD	2.22	1.39	1.33
13	A	814	CLA	C1A-NA	2.22	1.37	1.32
13	B	807	CLA	C3B-CAB	2.21	1.51	1.49
13	A	816	CLA	C4B-NB	2.21	1.37	1.34
13	A	812	CLA	C1A-NA	2.21	1.37	1.32
13	L	1002	CLA	O2D-CGD	2.21	1.39	1.33
13	A	843	CLA	C4B-NB	2.21	1.37	1.34
13	B	822	CLA	O2D-CGD	2.21	1.39	1.33
15	J	1104	BCR	C40-C30	-2.21	1.48	1.53
13	B	811	CLA	C4B-NB	2.21	1.37	1.34
15	L	1006	BCR	C20-C19	2.21	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	827	CLA	C3B-CAB	2.21	1.51	1.49
13	A	817	CLA	C3B-CAB	2.21	1.51	1.49
13	B	817	CLA	C4B-NB	2.21	1.37	1.34
13	L	1003	CLA	O2D-CGD	2.21	1.39	1.33
13	B	812	CLA	C4B-NB	2.20	1.37	1.34
13	B	831	CLA	C4D-C3D	-2.20	1.38	1.41
15	A	848	BCR	C40-C30	-2.20	1.48	1.53
15	A	851	BCR	C40-C30	-2.20	1.48	1.53
13	A	811	CLA	C5-C3	2.20	1.56	1.51
13	A	808	CLA	C4B-NB	2.20	1.37	1.34
13	B	838	CLA	O2D-CGD	2.20	1.39	1.33
13	A	809	CLA	C5-C3	2.20	1.56	1.51
13	A	842	CLA	C1A-NA	2.20	1.37	1.32
13	B	804	CLA	C4B-NB	2.20	1.37	1.34
15	A	850	BCR	C40-C30	-2.20	1.48	1.53
13	M	1201	CLA	C5-C3	2.20	1.56	1.51
15	B	846	BCR	C40-C30	-2.20	1.48	1.53
13	B	808	CLA	O2D-CGD	2.20	1.39	1.33
13	B	827	CLA	C5-C3	2.20	1.56	1.51
13	A	808	CLA	C5-C3	2.20	1.56	1.51
13	F	1301	CLA	C3D-CAD	-2.20	1.42	1.47
15	M	1203	BCR	C10-C9	2.20	1.38	1.35
13	M	1201	CLA	C1A-NA	2.19	1.37	1.32
13	B	803	CLA	O2D-CGD	2.19	1.38	1.33
15	B	850	BCR	C20-C19	2.19	1.40	1.34
15	B	850	BCR	C40-C30	-2.19	1.48	1.53
15	B	843	BCR	C20-C19	2.19	1.40	1.34
13	A	837	CLA	C4D-C3D	-2.19	1.38	1.41
13	B	825	CLA	C3B-CAB	2.19	1.51	1.49
13	B	839	CLA	C1A-NA	2.19	1.37	1.32
13	A	844	CLA	C4B-NB	2.19	1.37	1.34
13	A	804	CLA	C5-C3	2.19	1.56	1.51
13	A	801	CLA	C4B-NB	2.19	1.37	1.34
15	B	849	BCR	C40-C30	-2.19	1.48	1.53
13	B	829	CLA	C4D-C3D	-2.19	1.38	1.41
13	B	803	CLA	C5-C3	2.18	1.56	1.51
13	B	838	CLA	C5-C3	2.18	1.56	1.51
13	B	807	CLA	C1A-NA	2.18	1.37	1.32
13	B	806	CLA	C1A-NA	2.18	1.37	1.32
15	A	848	BCR	C20-C19	2.18	1.40	1.34
13	A	801	CLA	O2D-CGD	2.18	1.38	1.33
13	A	827	CLA	C4B-NB	2.18	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	828	CLA	C3D-CAD	-2.18	1.42	1.47
15	A	851	BCR	C20-C19	2.18	1.40	1.34
13	I	101	CLA	CBD-CAD	-2.18	1.46	1.56
13	B	805	CLA	C3B-CAB	2.18	1.51	1.49
13	A	831	CLA	C1A-NA	2.18	1.37	1.32
13	A	855	CLA	C4B-NB	2.18	1.37	1.34
15	J	1104	BCR	C20-C19	2.18	1.40	1.34
13	A	801	CLA	C5-C3	2.18	1.56	1.51
13	A	838	CLA	C4B-NB	2.18	1.37	1.34
13	B	816	CLA	C4B-NB	2.17	1.37	1.34
15	B	843	BCR	C8-C7	2.17	1.39	1.32
13	B	825	CLA	C3D-CAD	-2.17	1.42	1.47
13	A	811	CLA	O2D-CGD	2.17	1.38	1.33
13	A	843	CLA	C4D-C3D	-2.17	1.39	1.41
13	B	802	CLA	C4B-NB	2.17	1.37	1.34
13	B	822	CLA	C5-C3	2.17	1.56	1.51
15	A	847	BCR	C40-C30	-2.17	1.48	1.53
13	A	838	CLA	C1A-NA	2.17	1.37	1.32
15	A	849	BCR	C40-C30	-2.17	1.48	1.53
13	B	833	CLA	C3B-CAB	2.17	1.51	1.49
13	A	836	CLA	C1A-NA	2.17	1.37	1.32
13	A	809	CLA	C3D-CAD	-2.17	1.42	1.47
13	B	825	CLA	C5-C3	2.16	1.56	1.51
13	B	817	CLA	C1A-NA	2.16	1.37	1.32
13	J	1101	CLA	C4B-NB	2.16	1.37	1.34
13	A	831	CLA	O2D-CGD	2.16	1.38	1.33
13	A	826	CLA	C5-C3	2.16	1.56	1.51
13	A	835	CLA	C5-C3	2.16	1.56	1.51
13	B	836	CLA	C1A-NA	2.16	1.37	1.32
13	A	843	CLA	C3B-CAB	2.16	1.51	1.49
15	B	841	BCR	C40-C30	-2.16	1.48	1.53
13	A	819	CLA	C4B-NB	2.16	1.37	1.34
15	M	1203	BCR	C20-C19	2.15	1.40	1.34
15	A	849	BCR	C10-C9	2.15	1.38	1.35
13	B	820	CLA	C3B-CAB	2.15	1.51	1.49
13	A	837	CLA	C4B-NB	2.15	1.37	1.34
15	A	850	BCR	C11-C12	2.15	1.40	1.34
13	A	811	CLA	C3D-CAD	-2.15	1.43	1.47
13	B	824	CLA	C5-C3	2.15	1.56	1.51
13	A	831	CLA	C3B-C2B	-2.15	1.37	1.41
13	A	834	CLA	CHB-C4A	-2.15	1.31	1.36
13	A	842	CLA	CBD-CAD	-2.15	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	837	CLA	C1A-NA	2.14	1.37	1.32
15	L	1006	BCR	C40-C30	-2.14	1.48	1.53
13	B	817	CLA	C5-C3	2.14	1.56	1.51
13	J	1101	CLA	C3B-CAB	2.14	1.51	1.49
13	A	840	CLA	C3D-CAD	-2.14	1.43	1.47
13	A	827	CLA	C5-C3	2.14	1.56	1.51
13	B	839	CLA	C5-C3	2.14	1.56	1.51
15	L	1005	BCR	C20-C19	2.14	1.40	1.34
15	B	845	BCR	C20-C19	2.14	1.40	1.34
15	F	1302	BCR	C40-C30	-2.14	1.48	1.53
13	A	824	CLA	C4B-NB	2.14	1.37	1.34
15	B	842	BCR	C20-C19	2.14	1.40	1.34
13	B	803	CLA	C3B-C2B	-2.14	1.37	1.41
13	L	1002	CLA	C1A-NA	2.14	1.36	1.32
15	J	1104	BCR	C8-C7	2.14	1.39	1.32
13	A	835	CLA	C3B-CAB	2.14	1.51	1.49
13	A	824	CLA	C5-C3	2.13	1.56	1.51
13	B	801	CLA	C3B-CAB	2.13	1.51	1.49
13	I	101	CLA	C5-C3	2.13	1.56	1.51
13	B	836	CLA	CBD-CAD	-2.13	1.46	1.56
15	A	852	BCR	C40-C30	-2.13	1.49	1.53
13	A	808	CLA	CBD-CAD	-2.13	1.46	1.56
15	F	1302	BCR	C8-C7	2.13	1.39	1.32
13	B	837	CLA	C3B-CAB	2.13	1.51	1.49
13	A	822	CLA	C1A-NA	2.13	1.36	1.32
13	B	826	CLA	CBD-CAD	-2.13	1.46	1.56
13	A	832	CLA	C1A-NA	2.13	1.36	1.32
13	B	815	CLA	C5-C3	2.13	1.56	1.51
15	B	849	BCR	C20-C19	2.13	1.40	1.34
13	A	824	CLA	O2D-CGD	2.12	1.38	1.33
13	B	817	CLA	C3D-CAD	-2.12	1.43	1.47
13	B	831	CLA	C3D-CAD	-2.12	1.43	1.47
13	J	1102	CLA	C3B-CAB	2.12	1.51	1.49
13	B	821	CLA	C1A-NA	2.12	1.36	1.32
13	B	806	CLA	C5-C3	2.12	1.56	1.51
15	B	847	BCR	C20-C19	2.12	1.40	1.34
13	B	806	CLA	CBD-CAD	-2.12	1.46	1.56
15	B	849	BCR	C10-C9	2.12	1.38	1.35
13	I	101	CLA	C4B-NB	2.12	1.37	1.34
13	B	807	CLA	C4D-C3D	-2.12	1.39	1.41
13	B	820	CLA	C5-C3	2.12	1.56	1.51
13	B	836	CLA	C5-C3	2.12	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	816	CLA	C1A-NA	2.11	1.36	1.32
15	M	1203	BCR	C5-C6	2.11	1.37	1.34
15	A	847	BCR	C20-C19	2.11	1.40	1.34
13	L	1004	CLA	C5-C3	2.11	1.56	1.51
13	J	1103	CLA	C4B-NB	2.11	1.37	1.34
13	B	838	CLA	CBD-CAD	-2.11	1.46	1.56
13	B	831	CLA	C5-C3	2.11	1.56	1.51
13	B	829	CLA	C3B-CAB	2.11	1.51	1.49
13	A	815	CLA	C4B-NB	2.10	1.37	1.34
13	B	838	CLA	C4B-NB	2.10	1.37	1.34
13	M	1201	CLA	CBD-CAD	-2.10	1.46	1.56
13	A	824	CLA	C1A-NA	2.10	1.36	1.32
13	A	830	CLA	C4D-C3D	-2.10	1.39	1.41
15	A	850	BCR	C24-C25	2.10	1.53	1.46
13	J	1101	CLA	C5-C3	2.10	1.56	1.51
13	A	840	CLA	C3B-CAB	2.10	1.51	1.49
15	B	846	BCR	C39-C30	-2.10	1.49	1.53
13	B	806	CLA	C3B-CAB	2.10	1.51	1.49
13	M	1202	CLA	C3D-CAD	-2.10	1.43	1.47
13	A	822	CLA	C4D-C3D	-2.10	1.39	1.41
13	B	831	CLA	CBD-CAD	-2.10	1.46	1.56
13	F	1301	CLA	C4B-NB	2.10	1.37	1.34
13	B	807	CLA	C5-C3	2.09	1.56	1.51
13	A	828	CLA	C5-C3	2.09	1.56	1.51
13	X	102	CLA	C3B-CAB	2.09	1.51	1.49
13	A	833	CLA	C5-C3	2.09	1.56	1.51
15	L	1006	BCR	C8-C7	2.09	1.39	1.32
15	B	841	BCR	C20-C19	2.09	1.40	1.34
15	B	846	BCR	C20-C19	2.09	1.40	1.34
13	A	819	CLA	C5-C3	2.09	1.56	1.51
13	A	810	CLA	C3B-CAB	2.09	1.51	1.49
13	B	827	CLA	C3B-CAB	2.09	1.51	1.49
15	J	1105	BCR	C39-C30	-2.09	1.49	1.53
13	B	822	CLA	C4B-NB	2.09	1.37	1.34
13	A	830	CLA	C4B-NB	2.09	1.37	1.34
15	A	847	BCR	C8-C7	2.08	1.39	1.32
13	A	811	CLA	CBD-CAD	-2.08	1.46	1.56
13	A	814	CLA	CBD-CAD	-2.08	1.46	1.56
13	B	815	CLA	C3D-CAD	-2.08	1.43	1.47
13	B	817	CLA	CBD-CAD	-2.08	1.46	1.56
13	B	811	CLA	C3B-CAB	2.08	1.51	1.49
13	A	818	CLA	C5-C3	2.08	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	814	CLA	C4B-NB	2.08	1.37	1.34
13	A	814	CLA	C3D-CAD	-2.08	1.43	1.47
13	B	822	CLA	C3D-CAD	-2.08	1.43	1.47
13	A	822	CLA	CBD-CAD	-2.08	1.46	1.56
13	B	813	CLA	MG-NB	-2.08	2.00	2.05
15	A	847	BCR	C24-C25	2.07	1.53	1.46
13	B	808	CLA	C3B-CAB	2.07	1.51	1.49
13	B	826	CLA	C3B-C2B	-2.07	1.37	1.41
13	B	826	CLA	C1A-NA	2.07	1.36	1.32
13	I	101	CLA	C1A-NA	2.07	1.36	1.32
13	B	829	CLA	CBD-CAD	-2.07	1.47	1.56
15	L	1005	BCR	C8-C7	2.07	1.39	1.32
13	A	841	CLA	C3B-CAB	2.07	1.51	1.49
15	J	1104	BCR	C24-C25	2.07	1.53	1.46
13	A	824	CLA	CHB-C4A	-2.07	1.31	1.36
13	M	1201	CLA	C3B-CAB	2.07	1.51	1.49
13	B	802	CLA	C5-C3	2.07	1.56	1.51
13	J	1103	CLA	C1A-NA	2.07	1.36	1.32
15	A	851	BCR	C39-C30	-2.07	1.49	1.53
13	A	840	CLA	C5-C3	2.07	1.56	1.51
15	B	844	BCR	C39-C30	-2.07	1.49	1.53
15	A	852	BCR	C11-C12	2.06	1.40	1.34
13	A	819	CLA	C3B-CAB	2.06	1.51	1.49
13	B	836	CLA	C1A-CHA	-2.06	1.34	1.43
15	A	847	BCR	C11-C12	2.06	1.40	1.34
13	A	801	CLA	C3B-CAB	2.06	1.51	1.49
15	A	851	BCR	C8-C7	2.06	1.39	1.32
15	B	842	BCR	C24-C25	2.06	1.53	1.46
13	A	819	CLA	C1A-NA	2.06	1.36	1.32
13	A	830	CLA	CBD-CAD	-2.06	1.47	1.56
13	B	804	CLA	C5-C3	2.06	1.56	1.51
15	B	847	BCR	C8-C7	2.06	1.39	1.32
15	B	842	BCR	C11-C12	2.06	1.40	1.34
13	L	1002	CLA	CBD-CAD	-2.06	1.47	1.56
15	F	1302	BCR	C20-C19	2.06	1.40	1.34
13	A	820	CLA	CBD-CAD	-2.06	1.47	1.56
15	B	841	BCR	C24-C25	2.06	1.53	1.46
13	A	835	CLA	C1A-NA	2.06	1.36	1.32
13	B	810	CLA	C1A-NA	2.06	1.36	1.32
13	B	820	CLA	CBD-CAD	-2.05	1.47	1.56
13	B	823	CLA	C3B-CAB	2.05	1.51	1.49
13	A	819	CLA	C1A-CHA	-2.05	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	820	CLA	C5-C3	2.05	1.56	1.51
15	B	847	BCR	C39-C30	-2.05	1.49	1.53
13	A	812	CLA	C5-C3	2.05	1.56	1.51
15	B	841	BCR	C11-C12	2.05	1.40	1.34
13	A	818	CLA	C3D-CAD	-2.04	1.43	1.47
13	A	825	CLA	CBD-CAD	-2.05	1.47	1.56
15	I	102	BCR	C10-C9	2.04	1.38	1.35
13	B	814	CLA	CBD-CAD	-2.04	1.47	1.56
13	A	820	CLA	C4B-NB	2.04	1.37	1.34
13	L	1003	CLA	C4B-NB	2.04	1.37	1.34
13	A	838	CLA	C3D-CAD	-2.04	1.43	1.47
15	A	852	BCR	C24-C25	2.04	1.53	1.46
15	L	1005	BCR	C39-C30	-2.04	1.49	1.53
15	M	1203	BCR	C39-C30	-2.04	1.49	1.53
13	A	837	CLA	CBD-CAD	-2.04	1.47	1.56
13	A	816	CLA	C3B-CAB	2.04	1.51	1.49
13	B	814	CLA	C9-C8	-2.04	1.50	1.53
13	A	842	CLA	C1A-CHA	-2.04	1.34	1.43
13	A	802	CLA	CBD-CAD	-2.04	1.47	1.56
13	B	827	CLA	CBD-CAD	-2.04	1.47	1.56
13	A	843	CLA	CBD-CAD	-2.04	1.47	1.56
13	A	818	CLA	C3B-CAB	2.04	1.51	1.49
13	A	825	CLA	C3B-CAB	2.04	1.51	1.49
13	B	834	CLA	C3D-CAD	-2.04	1.43	1.47
15	B	841	BCR	C8-C7	2.04	1.38	1.32
13	A	834	CLA	CBD-CAD	-2.03	1.47	1.56
13	A	810	CLA	CBD-CAD	-2.03	1.47	1.56
15	B	846	BCR	C11-C12	2.03	1.40	1.34
15	J	1105	BCR	C11-C12	2.03	1.40	1.34
15	L	1005	BCR	C24-C25	2.03	1.53	1.46
15	B	847	BCR	C11-C12	2.03	1.40	1.34
13	A	802	CLA	C5-C3	2.03	1.56	1.51
15	B	841	BCR	C39-C30	-2.03	1.49	1.53
13	B	808	CLA	C5-C3	2.03	1.56	1.51
15	B	850	BCR	C11-C12	2.03	1.40	1.34
13	A	803	CLA	C5-C3	2.03	1.56	1.51
13	B	805	CLA	C5-C3	2.03	1.56	1.51
15	A	848	BCR	C11-C12	2.03	1.40	1.34
13	B	804	CLA	CBD-CAD	-2.03	1.47	1.56
13	A	832	CLA	CBD-CAD	-2.03	1.47	1.56
13	A	802	CLA	C1A-CHA	-2.03	1.34	1.43
13	B	822	CLA	CBD-CAD	-2.03	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	1104	BCR	C11-C12	2.03	1.40	1.34
13	A	812	CLA	CBD-CAD	-2.03	1.47	1.56
13	B	817	CLA	C1A-CHA	-2.02	1.34	1.43
13	A	826	CLA	C3D-CAD	-2.02	1.43	1.47
13	A	817	CLA	CBD-CAD	-2.02	1.47	1.56
15	B	843	BCR	C11-C12	2.02	1.40	1.34
13	B	837	CLA	CBD-CAD	-2.02	1.47	1.56
13	A	845	CLA	C5-C3	2.02	1.56	1.51
13	A	813	CLA	C5-C3	2.02	1.56	1.51
13	L	1003	CLA	C5-C3	2.02	1.56	1.51
15	A	847	BCR	C39-C30	-2.02	1.49	1.53
13	A	840	CLA	CBD-CAD	-2.02	1.47	1.56
13	A	833	CLA	C3B-CAB	2.02	1.51	1.49
13	A	833	CLA	CBD-CAD	-2.02	1.47	1.56
13	A	819	CLA	CBD-CAD	-2.02	1.47	1.56
13	B	823	CLA	CBD-CAD	-2.02	1.47	1.56
13	J	1103	CLA	C3B-C2B	-2.02	1.37	1.41
13	A	802	CLA	C1A-NA	2.01	1.36	1.32
15	L	1006	BCR	C11-C12	2.01	1.40	1.34
15	J	1105	BCR	C8-C7	2.01	1.38	1.32
13	A	829	CLA	CBD-CAD	-2.01	1.47	1.56
13	B	832	CLA	CBD-CAD	-2.01	1.47	1.56
13	B	827	CLA	O2D-CGD	2.01	1.38	1.33
15	F	1302	BCR	C39-C30	-2.01	1.49	1.53
13	B	820	CLA	O2A-C1	-2.01	1.39	1.46
13	A	821	CLA	CBD-CAD	-2.01	1.47	1.56
13	A	825	CLA	C3D-CAD	-2.01	1.43	1.47
13	A	817	CLA	C5-C3	2.01	1.56	1.51
13	A	806	CLA	C5-C3	2.01	1.56	1.51
13	A	801	CLA	C3D-CAD	-2.01	1.43	1.47
15	B	846	BCR	C8-C7	2.01	1.38	1.32
15	B	845	BCR	C24-C25	2.01	1.53	1.46
15	A	848	BCR	C39-C30	-2.01	1.49	1.53
13	A	820	CLA	C1A-CHA	-2.01	1.34	1.43
13	B	803	CLA	CBD-CAD	-2.01	1.47	1.56
15	B	845	BCR	C8-C7	2.01	1.38	1.32
13	B	810	CLA	CBD-CAD	-2.01	1.47	1.56
13	B	819	CLA	C3B-C2B	-2.01	1.37	1.41
13	B	812	CLA	C5-C3	2.00	1.56	1.51
15	A	851	BCR	C11-C12	2.00	1.39	1.34
13	B	821	CLA	CBD-CAD	-2.00	1.47	1.56
15	A	850	BCR	C8-C7	2.00	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	814	CLA	C3D-CAD	-2.00	1.43	1.47
13	B	818	CLA	CBD-CAD	-2.00	1.47	1.56
13	B	833	CLA	CBD-CAD	-2.00	1.47	1.56
13	A	855	CLA	C3B-CAB	2.00	1.51	1.49
13	M	1201	CLA	C1A-CHA	-2.00	1.34	1.43
13	B	835	CLA	CBD-CAD	-2.00	1.47	1.56
13	B	808	CLA	CBD-CAD	-2.00	1.47	1.56
15	L	1005	BCR	C11-C12	2.00	1.39	1.34

All (2027) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	824	CLA	C3D-CAD-CBD	-8.86	95.07	107.60
13	B	831	CLA	C3D-CAD-CBD	-8.27	95.90	107.60
13	A	844	CLA	CHA-CBD-CAD	-8.23	102.11	109.72
13	B	835	CLA	C3D-CAD-CBD	-7.74	96.65	107.60
13	J	1103	CLA	CHA-CBD-CAD	-7.62	102.67	109.72
13	A	801	CLA	C3D-CAD-CBD	-7.62	96.83	107.60
15	A	852	BCR	C15-C14-C13	-7.44	116.57	127.29
13	X	102	CLA	C3D-CAD-CBD	-7.40	97.14	107.60
13	X	102	CLA	O2D-CGD-CBD	7.37	126.35	111.33
13	B	802	CLA	O2D-CGD-CBD	7.34	126.28	111.33
13	A	837	CLA	C3D-CAD-CBD	-7.34	97.22	107.60
13	A	822	CLA	O2D-CGD-CBD	7.31	126.23	111.33
13	B	831	CLA	O2D-CGD-CBD	7.29	126.18	111.33
13	B	831	CLA	C4D-CHA-CBD	-7.10	92.66	109.37
15	B	849	BCR	C15-C14-C13	-7.09	117.08	127.29
13	A	824	CLA	C4D-CHA-CBD	-6.99	92.90	109.37
13	L	1003	CLA	C3D-CAD-CBD	-6.98	97.72	107.60
13	B	827	CLA	C3D-CAD-CBD	-6.92	97.82	107.60
13	B	817	CLA	O2D-CGD-CBD	6.81	125.19	111.33
15	B	844	BCR	C15-C14-C13	-6.76	119.01	127.61
13	A	814	CLA	C3D-CAD-CBD	-6.75	98.05	107.60
13	A	808	CLA	O2D-CGD-CBD	6.66	124.90	111.33
13	A	812	CLA	O2D-CGD-CBD	6.65	124.87	111.33
13	A	840	CLA	O2D-CGD-CBD	6.63	124.83	111.33
13	A	832	CLA	O2D-CGD-CBD	6.60	124.77	111.33
13	A	801	CLA	C4D-CHA-CBD	-6.56	93.92	109.37
13	A	837	CLA	C4D-CHA-CBD	-6.55	93.94	109.37
13	B	835	CLA	C4D-CHA-CBD	-6.54	93.97	109.37
13	A	824	CLA	O2D-CGD-CBD	6.52	124.61	111.33
13	A	822	CLA	C3D-CAD-CBD	-6.48	98.44	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	1102	CLA	C3D-CAD-CBD	-6.47	98.45	107.60
16	A	854	LHG	O8-C23-C24	6.46	120.08	111.94
13	B	824	CLA	C3D-CAD-CBD	-6.45	98.48	107.60
13	A	821	CLA	O2D-CGD-CBD	6.43	124.43	111.33
13	B	819	CLA	C3D-CAD-CBD	-6.37	98.59	107.60
13	A	811	CLA	O2D-CGD-CBD	6.35	124.26	111.33
13	A	834	CLA	C3B-CAB-CBB	-6.34	112.81	125.95
13	B	833	CLA	O2D-CGD-CBD	6.33	124.22	111.33
13	M	1201	CLA	O2D-CGD-CBD	6.32	124.21	111.33
13	X	102	CLA	C4D-CHA-CBD	-6.31	94.50	109.37
13	A	819	CLA	O2D-CGD-CBD	6.30	124.16	111.33
13	B	807	CLA	O2D-CGD-CBD	6.28	124.12	111.33
13	B	813	CLA	O2D-CGD-CBD	6.27	124.10	111.33
13	A	830	CLA	C3D-CAD-CBD	-6.25	98.76	107.60
13	B	808	CLA	O2D-CGD-CBD	6.20	123.95	111.33
13	B	811	CLA	C3D-CAD-CBD	-6.19	98.84	107.60
13	A	810	CLA	C3D-CAD-CBD	-6.17	98.87	107.60
13	B	812	CLA	O2D-CGD-CBD	6.17	123.89	111.33
13	B	822	CLA	O2D-CGD-CBD	6.14	123.83	111.33
13	L	1002	CLA	C3D-CAD-CBD	-6.12	98.95	107.60
13	B	827	CLA	O2D-CGD-CBD	6.11	123.78	111.33
13	A	810	CLA	O2D-CGD-CBD	6.11	123.77	111.33
13	A	801	CLA	O2D-CGD-CBD	6.10	123.76	111.33
13	B	821	CLA	C3D-CAD-CBD	-6.02	99.08	107.60
13	A	839	CLA	O2D-CGD-CBD	6.02	123.59	111.33
13	B	827	CLA	C4D-CHA-CBD	-6.01	95.22	109.37
13	B	809	CLA	C3D-CAD-CBD	-6.00	99.11	107.60
13	B	819	CLA	C4D-CHA-CBD	-5.99	95.26	109.37
13	B	814	CLA	O2D-CGD-CBD	5.97	123.48	111.33
15	A	850	BCR	C7-C8-C9	-5.95	117.31	126.22
13	B	809	CLA	O2D-CGD-CBD	5.94	123.43	111.33
13	B	802	CLA	C4D-CHA-CBD	-5.88	95.53	109.37
13	B	801	CLA	C3D-CAD-CBD	-5.87	99.30	107.60
13	L	1003	CLA	C4D-CHA-CBD	-5.86	95.57	109.37
13	J	1102	CLA	C4D-CHA-CBD	-5.86	95.58	109.37
13	B	824	CLA	O2D-CGD-CBD	5.85	123.25	111.33
13	A	814	CLA	C4D-CHA-CBD	-5.85	95.59	109.37
13	B	828	CLA	C3D-CAD-CBD	-5.85	99.33	107.60
13	L	1003	CLA	O2D-CGD-CBD	5.85	123.24	111.33
13	A	830	CLA	C4D-CHA-CBD	-5.83	95.63	109.37
13	B	832	CLA	C3D-CAD-CBD	-5.83	99.35	107.60
13	A	829	CLA	O2D-CGD-CBD	5.83	123.21	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	811	CLA	O2D-CGD-CBD	5.83	123.19	111.33
13	J	1102	CLA	O2D-CGD-CBD	5.82	123.19	111.33
13	A	837	CLA	CBD-CHA-C1A	5.79	136.34	128.77
13	B	803	CLA	C3D-CAD-CBD	-5.78	99.43	107.60
13	B	801	CLA	O2D-CGD-CBD	5.77	123.07	111.33
13	A	845	CLA	O2D-CGD-CBD	5.76	123.06	111.33
13	A	822	CLA	C4D-CHA-CBD	-5.75	95.83	109.37
13	A	815	CLA	O2D-CGD-CBD	5.75	123.04	111.33
13	A	813	CLA	O2D-CGD-CBD	5.74	123.02	111.33
13	A	810	CLA	C4D-CHA-CBD	-5.74	95.86	109.37
15	B	849	BCR	C11-C10-C9	-5.73	119.03	127.29
13	B	837	CLA	O2D-CGD-CBD	5.73	123.00	111.33
13	B	819	CLA	O2D-CGD-CBD	5.73	123.00	111.33
13	B	812	CLA	C4D-CHA-CBD	-5.72	95.90	109.37
13	B	809	CLA	C4D-CHA-CBD	-5.71	95.92	109.37
13	B	802	CLA	O1D-CGD-CBD	-5.69	112.77	124.42
13	L	1004	CLA	O2D-CGD-CBD	5.68	122.90	111.33
13	B	812	CLA	C3D-CAD-CBD	-5.68	99.57	107.60
13	B	811	CLA	C4D-CHA-CBD	-5.68	96.00	109.37
13	A	822	CLA	O1D-CGD-CBD	-5.66	112.82	124.42
13	A	808	CLA	C4D-CHA-CBD	-5.64	96.09	109.37
13	B	834	CLA	O2D-CGD-CBD	5.63	122.81	111.33
13	B	824	CLA	C4D-CHA-CBD	-5.63	96.11	109.37
13	B	803	CLA	C4D-CHA-CBD	-5.61	96.15	109.37
13	A	808	CLA	CGD-CBD-CHA	5.61	130.01	110.96
13	F	1301	CLA	O2D-CGD-CBD	5.60	122.75	111.33
13	J	1101	CLA	O2D-CGD-CBD	5.59	122.71	111.33
13	B	836	CLA	O2D-CGD-CBD	5.58	122.69	111.33
13	B	814	CLA	C4D-CHA-CBD	-5.58	96.23	109.37
13	L	1002	CLA	C4D-CHA-CBD	-5.57	96.24	109.37
13	A	855	CLA	O2D-CGD-CBD	5.57	122.68	111.33
13	B	814	CLA	C3D-CAD-CBD	-5.56	99.74	107.60
18	B	848	LMG	C30-C29-C28	5.56	135.30	113.51
13	A	805	CLA	O2D-CGD-CBD	5.56	122.64	111.33
13	B	828	CLA	C4D-CHA-CBD	-5.54	96.32	109.37
13	A	838	CLA	O2D-CGD-CBD	5.52	122.58	111.33
13	B	832	CLA	C4D-CHA-CBD	-5.52	96.37	109.37
13	A	825	CLA	O2D-CGD-CBD	5.52	122.57	111.33
13	L	1002	CLA	O2D-CGD-CBD	5.50	122.54	111.33
15	F	1302	BCR	C15-C14-C13	-5.50	119.38	127.29
13	A	809	CLA	CGD-CBD-CHA	5.48	129.60	110.96
13	B	830	CLA	O2D-CGD-CBD	5.47	122.48	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1202	CLA	O2D-CGD-CBD	5.45	122.44	111.33
13	B	828	CLA	O2D-CGD-CBD	5.43	122.39	111.33
13	A	816	CLA	C3D-CAD-CBD	-5.43	99.92	107.60
13	I	101	CLA	O2D-CGD-CBD	5.42	122.38	111.33
13	B	821	CLA	C4D-CHA-CBD	-5.39	96.68	109.37
13	B	801	CLA	C4D-CHA-CBD	-5.35	96.78	109.37
13	A	813	CLA	C3D-CAD-CBD	-5.33	100.06	107.60
13	A	818	CLA	O2D-CGD-CBD	5.33	122.18	111.33
15	B	845	BCR	C15-C14-C13	-5.30	119.66	127.29
13	A	843	CLA	O2D-CGD-CBD	5.29	122.11	111.33
13	A	828	CLA	C4D-CHA-CBD	-5.26	96.99	109.37
13	M	1202	CLA	C4D-CHA-CBD	-5.25	97.00	109.37
13	A	815	CLA	C3D-CAD-CBD	-5.25	100.17	107.60
13	B	834	CLA	C4D-CHA-CBD	-5.25	97.01	109.37
13	A	832	CLA	C3D-CAD-CBD	-5.24	100.19	107.60
13	A	808	CLA	C3D-CAD-CBD	-5.23	100.20	107.60
15	B	843	BCR	C3-C4-C5	5.22	121.65	113.74
13	A	843	CLA	C3D-CAD-CBD	-5.21	100.24	107.60
15	M	1203	BCR	C33-C5-C6	-5.20	118.61	124.51
15	B	845	BCR	C38-C26-C25	-5.20	118.61	124.51
13	B	803	CLA	O2D-CGD-CBD	5.20	121.91	111.33
13	B	832	CLA	O2D-CGD-CBD	5.19	121.91	111.33
13	A	836	CLA	O2D-CGD-CBD	5.19	121.90	111.33
13	X	102	CLA	O1D-CGD-CBD	-5.18	113.81	124.42
13	A	813	CLA	C4D-CHA-CBD	-5.15	97.23	109.37
13	B	804	CLA	O2D-CGD-CBD	5.16	121.83	111.33
13	B	839	CLA	O2D-CGD-CBD	5.14	121.81	111.33
13	B	802	CLA	C3D-CAD-CBD	-5.13	100.35	107.60
13	B	812	CLA	CGD-CBD-CHA	5.12	128.36	110.96
13	A	843	CLA	C4D-CHA-CBD	-5.11	97.34	109.37
13	B	808	CLA	C4D-CHA-CBD	-5.08	97.41	109.37
13	B	834	CLA	C3D-CAD-CBD	-5.08	100.42	107.60
13	A	827	CLA	C3D-CAD-CBD	-5.07	100.43	107.60
13	M	1202	CLA	CGD-CBD-CHA	5.07	128.19	110.96
13	A	828	CLA	O2D-CGD-CBD	5.05	121.61	111.33
13	B	837	CLA	C3D-CAD-CBD	-5.04	100.47	107.60
13	A	830	CLA	O2D-CGD-CBD	5.03	121.58	111.33
13	A	807	CLA	CGD-CBD-CHA	5.03	128.04	110.96
13	A	803	CLA	C3D-CAD-CBD	-5.02	100.50	107.60
15	B	847	BCR	C33-C5-C6	-5.01	118.82	124.51
13	B	838	CLA	O2D-CGD-CBD	5.01	121.53	111.33
15	B	850	BCR	C7-C8-C9	-5.00	118.73	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1202	CLA	C3D-CAD-CBD	-5.00	100.53	107.60
13	A	811	CLA	C4D-CHA-CBD	-5.00	97.61	109.37
13	A	816	CLA	C4D-CHA-CBD	-4.99	97.62	109.37
13	B	802	CLA	CGD-CBD-CHA	4.99	127.90	110.96
15	J	1104	BCR	C28-C27-C26	4.98	121.29	113.74
13	A	829	CLA	C4D-CHA-CBD	-4.98	97.65	109.37
13	B	837	CLA	C4D-CHA-CBD	-4.95	97.70	109.37
13	A	807	CLA	CED-O2D-CGD	4.95	127.80	116.02
13	A	817	CLA	C4D-CHA-CBD	-4.95	97.71	109.37
15	L	1005	BCR	C16-C17-C18	-4.95	120.16	127.29
13	B	831	CLA	CGD-CBD-CHA	4.94	127.75	110.96
13	A	855	CLA	C3D-CAD-CBD	-4.94	100.61	107.60
13	B	835	CLA	O2D-CGD-CBD	4.94	121.38	111.33
13	A	827	CLA	C4D-CHA-CBD	-4.93	97.75	109.37
13	A	809	CLA	C4D-CHA-CBD	-4.92	97.78	109.37
13	B	813	CLA	C4D-CHA-CBD	-4.91	97.80	109.37
13	A	832	CLA	C4D-CHA-CBD	-4.91	97.80	109.37
15	B	842	BCR	C15-C14-C13	-4.91	120.22	127.29
13	I	101	CLA	C4D-CHA-CBD	-4.89	97.85	109.37
13	A	809	CLA	O2D-CGD-CBD	4.89	121.30	111.33
15	B	842	BCR	C3-C4-C5	4.89	121.16	113.74
13	A	831	CLA	C4D-CHA-CBD	-4.89	97.85	109.37
13	A	855	CLA	C4D-CHA-CBD	-4.89	97.85	109.37
13	I	101	CLA	O1D-CGD-CBD	-4.88	114.42	124.42
13	B	818	CLA	C4D-CHA-CBD	-4.87	97.91	109.37
15	B	843	BCR	C2-C1-C6	4.86	118.51	110.44
13	B	818	CLA	C3D-CAD-CBD	-4.85	100.74	107.60
15	A	852	BCR	C33-C5-C6	-4.84	119.02	124.51
15	J	1104	BCR	C29-C30-C25	4.83	118.47	110.44
13	B	813	CLA	CBD-CHA-C1A	4.83	135.08	128.77
13	M	1201	CLA	C4D-CHA-CBD	-4.83	98.00	109.37
13	I	101	CLA	C3D-CAD-CBD	-4.83	100.78	107.60
13	A	803	CLA	C4D-CHA-CBD	-4.82	98.02	109.37
13	B	829	CLA	C4D-CHA-CBD	-4.82	98.03	109.37
13	B	819	CLA	CGD-CBD-CHA	4.81	127.30	110.96
13	B	808	CLA	C3D-CAD-CBD	-4.80	100.81	107.60
15	B	842	BCR	C33-C5-C6	-4.80	119.06	124.51
13	A	815	CLA	C4D-CHA-CBD	-4.80	98.07	109.37
13	B	816	CLA	O2D-CGD-CBD	4.80	121.10	111.33
13	B	813	CLA	C3D-CAD-CBD	-4.79	100.83	107.60
13	A	828	CLA	C3D-CAD-CBD	-4.78	100.83	107.60
13	B	838	CLA	C4D-CHA-CBD	-4.78	98.11	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	827	CLA	O2D-CGD-CBD	4.78	121.07	111.33
13	B	827	CLA	CGD-CBD-CHA	4.77	127.17	110.96
13	A	807	CLA	C4D-CHA-CBD	-4.77	98.14	109.37
15	B	845	BCR	C29-C30-C25	4.76	118.36	110.44
13	B	809	CLA	CGD-CBD-CHA	4.76	127.13	110.96
13	A	819	CLA	C4-C3-C5	4.75	122.62	115.39
15	M	1203	BCR	C3-C4-C5	4.76	120.95	113.74
15	B	850	BCR	C2-C1-C6	4.75	118.33	110.44
13	B	814	CLA	CGD-CBD-CHA	4.75	127.09	110.96
13	A	829	CLA	C3D-CAD-CBD	-4.75	100.89	107.60
15	B	845	BCR	C28-C27-C26	4.73	120.91	113.74
13	A	811	CLA	CGD-CBD-CHA	4.73	127.02	110.96
15	B	842	BCR	C2-C1-C6	4.72	118.28	110.44
13	B	807	CLA	C2D-C1D-ND	4.71	112.97	109.41
15	A	852	BCR	C15-C16-C17	-4.71	112.94	123.36
13	A	838	CLA	C4D-CHA-CBD	-4.70	98.29	109.37
13	A	840	CLA	C4D-CHA-CBD	-4.70	98.30	109.37
13	A	825	CLA	C4D-CHA-CBD	-4.70	98.30	109.37
13	B	823	CLA	O2D-CGD-CBD	4.70	120.90	111.33
13	A	837	CLA	O2D-CGD-CBD	4.70	120.89	111.33
13	A	810	CLA	CGD-CBD-CHA	4.69	126.91	110.96
13	A	845	CLA	C4D-CHA-CBD	-4.68	98.36	109.37
15	B	847	BCR	C2-C1-C6	4.68	118.21	110.44
15	B	850	BCR	C38-C26-C25	-4.67	119.21	124.51
13	B	827	CLA	C2D-C1D-ND	4.67	112.93	109.41
13	A	834	CLA	O2D-CGD-CBD	4.66	120.83	111.33
13	A	801	CLA	CGD-CBD-CHA	4.65	126.77	110.96
13	A	817	CLA	C3D-CAD-CBD	-4.65	101.02	107.60
13	A	826	CLA	C4D-CHA-CBD	-4.64	98.44	109.37
13	J	1102	CLA	CGD-CBD-CHA	4.62	126.68	110.96
13	A	838	CLA	C3D-CAD-CBD	-4.62	101.06	107.60
13	A	812	CLA	C4D-CHA-CBD	-4.62	98.49	109.37
13	A	828	CLA	CGD-CBD-CHA	4.59	126.58	110.96
13	A	809	CLA	C2D-C1D-ND	4.58	112.87	109.41
13	A	814	CLA	O2D-CGD-CBD	4.58	120.66	111.33
13	B	806	CLA	C4D-CHA-CBD	-4.57	98.60	109.37
13	A	807	CLA	C2D-C1D-ND	4.57	112.86	109.41
13	M	1201	CLA	C3D-CAD-CBD	-4.56	101.15	107.60
13	A	830	CLA	C2D-C1D-ND	4.56	112.85	109.41
13	A	845	CLA	C3D-CAD-CBD	-4.54	101.18	107.60
13	B	802	CLA	C1D-C2D-C3D	-4.53	103.08	106.78
13	F	1301	CLA	C4D-CHA-CBD	-4.52	98.73	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	850	BCR	C3-C4-C5	4.52	120.59	113.74
13	B	828	CLA	CGD-CBD-CHA	4.52	126.31	110.96
13	A	830	CLA	CGD-CBD-CHA	4.51	126.31	110.96
13	A	804	CLA	C4D-CHA-CBD	-4.51	98.76	109.37
13	B	816	CLA	C4D-CHA-CBD	-4.50	98.78	109.37
13	A	840	CLA	C2D-C1D-ND	4.50	112.81	109.41
15	A	851	BCR	C15-C14-C13	-4.49	120.82	127.29
13	B	806	CLA	C1-C2-C3	-4.49	118.20	126.19
15	I	102	BCR	C3-C4-C5	4.49	120.55	113.74
15	I	102	BCR	C33-C5-C6	-4.49	119.42	124.51
13	A	842	CLA	C4D-CHA-CBD	-4.49	98.81	109.37
13	B	806	CLA	O2D-CGD-CBD	4.49	120.47	111.33
15	M	1203	BCR	C2-C1-C6	4.49	117.90	110.44
13	A	802	CLA	O2D-CGD-CBD	4.49	120.47	111.33
15	I	102	BCR	C2-C1-C6	4.48	117.89	110.44
15	L	1006	BCR	C16-C17-C18	-4.48	120.84	127.29
13	A	831	CLA	C3D-CAD-CBD	-4.47	101.27	107.60
13	A	811	CLA	C3D-CAD-CBD	-4.47	101.28	107.60
13	A	826	CLA	C3D-CAD-CBD	-4.46	101.29	107.60
15	B	847	BCR	C3-C4-C5	4.46	120.49	113.74
13	B	813	CLA	CGD-CBD-CHA	4.45	126.09	110.96
13	A	807	CLA	C1D-C2D-C3D	-4.45	103.14	106.78
13	B	814	CLA	C2D-C1D-ND	4.45	112.77	109.41
13	A	840	CLA	C3D-CAD-CBD	-4.44	101.32	107.60
15	I	102	BCR	C38-C26-C25	-4.43	119.48	124.51
13	A	832	CLA	O2A-C1-C2	4.43	118.15	108.55
15	B	843	BCR	C16-C17-C18	-4.43	120.92	127.29
13	B	807	CLA	C4D-CHA-CBD	-4.42	98.96	109.37
13	A	840	CLA	O1D-CGD-CBD	-4.42	115.37	124.42
15	L	1005	BCR	C38-C26-C25	-4.42	119.50	124.51
15	A	849	BCR	C16-C17-C18	-4.41	120.94	127.29
13	B	802	CLA	C1-C2-C3	-4.41	118.35	126.19
13	A	837	CLA	C2D-C1D-ND	4.41	112.74	109.41
13	A	841	CLA	C4D-CHA-CBD	-4.40	99.00	109.37
13	I	101	CLA	C2D-C1D-ND	4.40	112.73	109.41
13	A	833	CLA	C4D-CHA-CBD	-4.39	99.03	109.37
13	M	1201	CLA	C2D-C1D-ND	4.38	112.72	109.41
13	B	808	CLA	CGD-CBD-CHA	4.38	125.86	110.96
15	B	850	BCR	C15-C14-C13	-4.38	120.98	127.29
15	B	843	BCR	C33-C5-C6	-4.38	119.54	124.51
13	B	822	CLA	C4D-CHA-CBD	-4.38	99.06	109.37
15	B	847	BCR	C16-C17-C18	-4.38	120.99	127.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	826	CLA	O2D-CGD-CBD	4.38	120.24	111.33
13	A	841	CLA	C3D-CAD-CBD	-4.37	101.42	107.60
15	F	1302	BCR	C33-C5-C6	-4.37	119.55	124.51
13	B	823	CLA	C4D-CHA-CBD	-4.37	99.09	109.37
13	A	818	CLA	O2A-C1-C2	-4.36	99.10	108.55
13	A	812	CLA	C3D-CAD-CBD	-4.36	101.44	107.60
13	M	1201	CLA	CGD-CBD-CHA	4.35	125.75	110.96
15	A	852	BCR	C38-C26-C25	-4.35	119.58	124.51
13	A	825	CLA	C3D-CAD-CBD	-4.35	101.45	107.60
13	B	838	CLA	C3D-CAD-CBD	-4.34	101.46	107.60
13	J	1101	CLA	C4D-CHA-CBD	-4.34	99.15	109.37
13	A	827	CLA	C2D-C1D-ND	4.34	112.68	109.41
13	B	825	CLA	C4D-CHA-CBD	-4.32	99.19	109.37
15	A	851	BCR	C38-C26-C25	-4.32	119.61	124.51
13	B	839	CLA	C4D-CHA-CBD	-4.32	99.20	109.37
13	B	829	CLA	C3D-CAD-CBD	-4.32	101.49	107.60
13	A	818	CLA	C1-O2A-CGA	4.31	129.04	116.98
13	B	806	CLA	C3D-CAD-CBD	-4.31	101.51	107.60
13	A	804	CLA	O2D-CGD-CBD	4.31	120.10	111.33
13	B	833	CLA	C4D-CHA-CBD	-4.31	99.23	109.37
15	J	1105	BCR	C38-C26-C25	-4.30	119.63	124.51
13	F	1301	CLA	CBD-CHA-C1A	4.30	134.39	128.77
13	A	832	CLA	O1D-CGD-CBD	-4.29	115.62	124.42
13	B	810	CLA	C4D-CHA-CBD	-4.29	99.26	109.37
13	A	806	CLA	C1-C2-C3	-4.28	118.57	126.19
13	B	822	CLA	CGD-CBD-CHA	4.28	125.52	110.96
13	A	837	CLA	C1D-C2D-C3D	-4.28	103.28	106.78
13	B	834	CLA	CGD-CBD-CHA	4.27	125.48	110.96
15	L	1006	BCR	C24-C23-C22	-4.27	119.82	126.22
13	A	845	CLA	CGD-CBD-CHA	4.27	125.46	110.96
15	A	850	BCR	C24-C23-C22	-4.26	119.84	126.22
15	A	851	BCR	C24-C23-C22	-4.26	119.85	126.22
13	B	838	CLA	CGD-CBD-CHA	4.26	125.43	110.96
13	A	805	CLA	C2D-C1D-ND	4.25	112.62	109.41
13	B	807	CLA	CGD-CBD-CHA	4.25	125.40	110.96
13	A	810	CLA	C2D-C1D-ND	4.24	112.61	109.41
15	F	1302	BCR	C11-C10-C9	-4.24	121.19	127.29
15	B	850	BCR	C16-C17-C18	-4.24	121.19	127.29
13	X	102	CLA	CGD-CBD-CHA	4.24	125.36	110.96
15	L	1006	BCR	C38-C26-C25	-4.23	119.70	124.51
13	A	809	CLA	C3D-CAD-CBD	-4.23	101.61	107.60
13	B	831	CLA	C2D-C1D-ND	4.22	112.59	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	1004	CLA	C4D-CHA-CBD	-4.22	99.44	109.37
13	M	1202	CLA	CBD-CHA-C1A	4.22	134.28	128.77
13	B	833	CLA	CGD-CBD-CHA	4.21	125.27	110.96
15	A	851	BCR	C33-C5-C6	-4.21	119.74	124.51
13	B	829	CLA	CGD-CBD-CHA	4.21	125.26	110.96
14	B	840	PQN	C11-C12-C13	-4.20	119.66	126.76
13	A	837	CLA	CGD-CBD-CHA	4.20	125.25	110.96
13	A	822	CLA	C2D-C1D-ND	4.20	112.58	109.41
13	A	804	CLA	CGD-CBD-CHA	4.19	125.19	110.96
13	A	805	CLA	C4D-CHA-CBD	-4.18	99.52	109.37
13	A	828	CLA	C2D-C1D-ND	4.18	112.56	109.41
15	B	849	BCR	C38-C26-C25	-4.17	119.78	124.51
13	B	816	CLA	C3D-CAD-CBD	-4.17	101.70	107.60
15	A	852	BCR	C38-C26-C27	4.16	120.97	113.34
15	B	843	BCR	C29-C30-C25	4.15	117.34	110.44
15	B	842	BCR	C24-C23-C22	-4.15	120.00	126.22
13	B	824	CLA	CGD-CBD-CHA	4.15	125.07	110.96
13	A	821	CLA	CGD-CBD-CHA	4.15	125.07	110.96
13	A	817	CLA	C2D-C1D-ND	4.14	112.54	109.41
15	L	1005	BCR	C33-C5-C6	-4.13	119.83	124.51
13	B	802	CLA	C2D-C1D-ND	4.13	112.53	109.41
13	B	804	CLA	C4D-CHA-CBD	-4.13	99.66	109.37
13	A	801	CLA	C2D-C1D-ND	4.11	112.52	109.41
15	J	1105	BCR	C38-C26-C27	4.11	120.88	113.34
13	B	836	CLA	C4D-CHA-CBD	-4.10	99.71	109.37
15	L	1005	BCR	C38-C26-C27	4.09	120.86	113.34
13	B	809	CLA	C2D-C1D-ND	4.09	112.50	109.41
13	A	818	CLA	C4D-CHA-CBD	-4.09	99.75	109.37
15	L	1005	BCR	C7-C8-C9	-4.09	120.10	126.22
15	A	848	BCR	C38-C26-C25	-4.09	119.87	124.51
13	B	818	CLA	C1-O2A-CGA	4.08	119.85	115.06
15	B	841	BCR	C16-C17-C18	-4.08	121.42	127.29
15	B	847	BCR	C38-C26-C25	-4.08	119.89	124.51
15	B	850	BCR	C11-C10-C9	-4.07	121.43	127.29
13	A	840	CLA	C1D-C2D-C3D	-4.07	103.46	106.78
15	J	1105	BCR	C33-C5-C6	-4.07	119.89	124.51
15	A	849	BCR	C20-C21-C22	-4.07	121.43	127.29
15	B	850	BCR	C38-C26-C27	4.06	120.79	113.34
15	A	848	BCR	C24-C23-C22	-4.06	120.14	126.22
13	A	829	CLA	C1-O2A-CGA	4.06	128.35	116.98
15	A	848	BCR	C33-C5-C6	-4.06	119.91	124.51
13	B	804	CLA	C2D-C1D-ND	4.06	112.47	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	806	CLA	C2D-C1D-ND	4.06	112.47	109.41
13	A	811	CLA	C2D-C1D-ND	4.05	112.47	109.41
13	L	1004	CLA	CGD-CBD-CHA	4.05	124.73	110.96
13	A	842	CLA	C3D-CAD-CBD	-4.04	101.89	107.60
15	J	1104	BCR	C38-C26-C25	-4.04	119.93	124.51
15	B	846	BCR	C16-C17-C18	-4.03	121.48	127.29
13	B	823	CLA	CGD-CBD-CHA	4.03	124.66	110.96
15	A	850	BCR	C38-C26-C25	-4.03	119.94	124.51
13	A	831	CLA	C2D-C1D-ND	4.03	112.45	109.41
15	B	841	BCR	C33-C5-C6	-4.03	119.94	124.51
13	A	826	CLA	CGD-CBD-CHA	4.03	124.64	110.96
15	J	1104	BCR	C33-C5-C6	-4.02	119.95	124.51
13	B	820	CLA	CGD-CBD-CHA	4.02	124.61	110.96
13	B	825	CLA	CGD-CBD-CHA	4.01	124.59	110.96
13	B	801	CLA	C2D-C1D-ND	4.01	112.44	109.41
13	A	808	CLA	C2D-C1D-ND	4.01	112.44	109.41
13	B	832	CLA	C2D-C1D-ND	4.01	112.44	109.41
13	A	819	CLA	C2D-C1D-ND	4.01	112.44	109.41
15	A	848	BCR	C38-C26-C27	4.01	120.70	113.34
13	M	1201	CLA	C1D-C2D-C3D	-4.01	103.51	106.78
13	B	805	CLA	C1-C2-C3	-4.01	119.06	126.19
13	A	843	CLA	C2D-C1D-ND	4.00	112.43	109.41
13	A	817	CLA	CGD-CBD-CHA	4.00	124.55	110.96
15	B	843	BCR	C23-C24-C25	-3.99	115.52	127.32
13	J	1101	CLA	CGD-CBD-CHA	3.99	124.52	110.96
15	I	102	BCR	C38-C26-C27	3.99	120.66	113.34
13	A	845	CLA	C2D-C1D-ND	3.98	112.42	109.41
13	A	835	CLA	O2D-CGD-CBD	3.98	119.44	111.33
15	B	845	BCR	C24-C23-C22	-3.98	120.26	126.22
13	A	814	CLA	C2D-C1D-ND	3.97	112.41	109.41
13	A	804	CLA	C2D-C1D-ND	3.97	112.41	109.41
13	A	819	CLA	C4D-CHA-CBD	-3.97	100.03	109.37
15	A	848	BCR	C7-C8-C9	-3.97	120.28	126.22
15	B	842	BCR	C11-C10-C9	-3.96	121.58	127.29
13	A	809	CLA	C1D-C2D-C3D	-3.96	103.54	106.78
13	B	833	CLA	C3D-CAD-CBD	-3.96	102.00	107.60
13	F	1301	CLA	C2D-C1D-ND	3.96	112.40	109.41
13	B	825	CLA	O2D-CGD-CBD	3.96	119.39	111.33
15	A	848	BCR	C16-C17-C18	-3.95	121.60	127.29
13	B	831	CLA	C1D-C2D-C3D	-3.95	103.55	106.78
15	B	843	BCR	C28-C27-C26	3.95	119.72	113.74
13	B	821	CLA	C2D-C1D-ND	3.94	112.39	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	829	CLA	CGD-CBD-CHA	3.95	124.37	110.96
13	I	101	CLA	C1D-C2D-C3D	-3.94	103.56	106.78
15	A	852	BCR	C33-C5-C4	3.94	120.57	113.34
13	A	829	CLA	CAA-CBA-CGA	-3.94	100.57	113.27
15	A	848	BCR	C33-C5-C4	3.94	120.56	113.34
13	A	803	CLA	C2D-C1D-ND	3.93	112.38	109.41
13	B	830	CLA	C2D-C1D-ND	3.93	112.38	109.41
15	B	844	BCR	C38-C26-C25	-3.92	120.06	124.51
15	B	841	BCR	C33-C5-C4	3.92	120.54	113.34
13	B	826	CLA	C2D-C1D-ND	3.92	112.37	109.41
13	B	831	CLA	O1D-CGD-CBD	-3.92	116.39	124.42
15	B	843	BCR	C38-C26-C25	-3.92	120.06	124.51
13	B	837	CLA	C2D-C1D-ND	3.92	112.37	109.41
15	J	1104	BCR	C7-C8-C9	-3.92	120.36	126.22
13	A	828	CLA	C1D-C2D-C3D	-3.91	103.58	106.78
13	A	820	CLA	C4D-CHA-CBD	-3.92	100.15	109.37
15	A	851	BCR	C38-C26-C27	3.91	120.52	113.34
13	B	812	CLA	O1D-CGD-CBD	-3.90	116.42	124.42
15	J	1104	BCR	C33-C5-C4	3.90	120.51	113.34
15	A	851	BCR	C16-C17-C18	-3.91	121.67	127.29
15	J	1105	BCR	C33-C5-C4	3.90	120.50	113.34
13	B	815	CLA	C2D-C1D-ND	3.90	112.36	109.41
13	B	832	CLA	CGD-CBD-CHA	3.90	124.22	110.96
15	A	849	BCR	C33-C5-C6	-3.90	120.09	124.51
13	B	837	CLA	CGD-CBD-CHA	3.90	124.21	110.96
13	B	810	CLA	C3D-CAD-CBD	-3.90	102.09	107.60
13	F	1301	CLA	C3D-CAD-CBD	-3.89	102.09	107.60
13	B	815	CLA	C4D-CHA-CBD	-3.89	100.20	109.37
15	M	1203	BCR	C38-C26-C27	3.89	120.49	113.34
13	A	806	CLA	C4D-CHA-CBD	-3.89	100.21	109.37
15	A	847	BCR	C16-C17-C18	-3.89	121.69	127.29
13	A	808	CLA	O2D-CGD-O1D	-3.89	115.89	123.79
13	A	809	CLA	C4A-NA-C1A	3.89	111.88	106.52
13	A	808	CLA	C1D-C2D-C3D	-3.88	103.61	106.78
13	A	816	CLA	CGD-CBD-CHA	3.88	124.16	110.96
15	A	850	BCR	C38-C26-C27	3.88	120.47	113.34
13	A	842	CLA	C4-C3-C5	3.88	121.29	115.39
13	B	835	CLA	C2D-C1D-ND	3.88	112.34	109.41
15	A	849	BCR	C7-C8-C9	-3.88	120.42	126.22
13	B	803	CLA	C2D-C1D-ND	3.87	112.33	109.41
13	B	808	CLA	C2D-C1D-ND	3.87	112.33	109.41
13	A	839	CLA	CGD-CBD-CHA	3.86	124.06	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	835	CLA	C1D-C2D-C3D	-3.85	103.63	106.78
15	L	1006	BCR	C38-C26-C27	3.85	120.41	113.34
13	A	808	CLA	C4A-NA-C1A	3.85	111.83	106.52
15	F	1302	BCR	C33-C5-C4	3.85	120.41	113.34
13	B	829	CLA	C2D-C1D-ND	3.85	112.32	109.41
13	A	804	CLA	C3D-CAD-CBD	-3.84	102.16	107.60
13	A	831	CLA	O2D-CGD-CBD	3.84	119.16	111.33
15	M	1203	BCR	C8-C7-C6	-3.84	115.97	127.32
15	L	1005	BCR	C33-C5-C4	3.84	120.39	113.34
15	I	102	BCR	C7-C8-C9	-3.84	120.47	126.22
13	A	833	CLA	CGD-CBD-CHA	3.84	124.00	110.96
15	B	850	BCR	C24-C23-C22	-3.84	120.47	126.22
13	A	830	CLA	C1D-C2D-C3D	-3.84	103.64	106.78
13	F	1301	CLA	CGD-CBD-CHA	3.83	123.99	110.96
13	A	804	CLA	C1D-C2D-C3D	-3.83	103.65	106.78
13	A	833	CLA	C1D-C2D-C3D	-3.83	103.65	106.78
13	B	815	CLA	CGD-CBD-CHA	3.83	123.98	110.96
13	A	838	CLA	C2D-C1D-ND	3.83	112.30	109.41
13	B	838	CLA	CAA-CBA-CGA	-3.83	100.92	113.27
15	B	846	BCR	C20-C21-C22	-3.83	121.78	127.29
13	B	826	CLA	C4D-CHA-CBD	-3.83	100.36	109.37
13	B	803	CLA	CGD-CBD-CHA	3.82	123.96	110.96
13	A	830	CLA	C4A-NA-C1A	3.82	111.79	106.52
13	A	826	CLA	CBD-CHA-C1A	3.82	133.76	128.77
13	A	820	CLA	C2D-C1D-ND	3.82	112.29	109.41
15	B	844	BCR	C38-C26-C27	3.82	120.34	113.34
13	A	818	CLA	CGD-CBD-CHA	3.81	123.90	110.96
13	A	812	CLA	C2D-C1D-ND	3.80	112.28	109.41
13	B	819	CLA	C2D-C1D-ND	3.80	112.28	109.41
13	A	834	CLA	C2D-C1D-ND	3.80	112.28	109.41
13	A	833	CLA	C2D-C1D-ND	3.80	112.28	109.41
13	B	814	CLA	C1D-C2D-C3D	-3.80	103.67	106.78
13	M	1202	CLA	C2D-C1D-ND	3.80	112.28	109.41
15	B	849	BCR	C33-C5-C4	3.80	120.32	113.34
16	A	854	LHG	O7-C7-C8	3.80	119.88	111.56
13	A	816	CLA	C2D-C1D-ND	3.80	112.28	109.41
15	L	1005	BCR	C24-C23-C22	-3.80	120.54	126.22
13	B	816	CLA	C2D-C1D-ND	3.79	112.28	109.41
13	A	813	CLA	CGD-CBD-CHA	3.79	123.85	110.96
13	M	1202	CLA	C4A-NA-C1A	3.79	111.75	106.52
13	A	839	CLA	C1-O2A-CGA	3.79	119.51	115.06
13	A	831	CLA	C1D-C2D-C3D	-3.79	103.68	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	849	BCR	C38-C26-C27	3.79	120.30	113.34
15	B	847	BCR	C38-C26-C27	3.79	120.30	113.34
13	A	823	CLA	C2D-C1D-ND	3.79	112.27	109.41
15	A	847	BCR	C33-C5-C6	-3.79	120.21	124.51
13	B	801	CLA	CGD-CBD-CHA	3.79	123.83	110.96
13	F	1301	CLA	C1D-C2D-C3D	-3.79	103.69	106.78
13	B	827	CLA	C4A-NA-C1A	3.78	111.74	106.52
15	B	842	BCR	C20-C21-C22	-3.78	121.84	127.29
13	J	1101	CLA	C3D-CAD-CBD	-3.78	102.25	107.60
13	A	819	CLA	O1D-CGD-CBD	-3.78	116.67	124.42
13	A	838	CLA	C1D-C2D-C3D	-3.78	103.69	106.78
13	B	820	CLA	C4D-CHA-CBD	-3.78	100.47	109.37
13	A	839	CLA	C4A-NA-C1A	3.78	111.73	106.52
13	A	842	CLA	CGD-CBD-CHA	3.78	123.80	110.96
13	A	839	CLA	C2D-C1D-ND	3.78	112.26	109.41
13	A	819	CLA	C4A-NA-C1A	3.78	111.73	106.52
16	A	853	LHG	O7-C7-C8	3.78	119.83	111.56
13	A	819	CLA	CGD-CBD-CHA	3.77	123.78	110.96
13	A	825	CLA	C2D-C1D-ND	3.77	112.26	109.41
15	A	849	BCR	C38-C26-C25	-3.76	120.24	124.51
13	B	836	CLA	CGD-CBD-CHA	3.76	123.76	110.96
13	L	1002	CLA	C2D-C1D-ND	3.77	112.25	109.41
13	A	822	CLA	C1D-C2D-C3D	-3.76	103.70	106.78
13	A	814	CLA	C1D-C2D-C3D	-3.76	103.70	106.78
13	B	820	CLA	C2D-C1D-ND	3.76	112.25	109.41
15	B	842	BCR	C38-C26-C25	-3.76	120.24	124.51
13	A	820	CLA	O2D-CGD-CBD	3.76	118.99	111.33
13	A	801	CLA	C1D-C2D-C3D	-3.76	103.71	106.78
15	B	846	BCR	C33-C5-C6	-3.76	120.25	124.51
15	B	849	BCR	C38-C26-C27	3.76	120.23	113.34
15	A	847	BCR	C2-C1-C6	3.75	116.68	110.44
13	B	807	CLA	C1D-C2D-C3D	-3.75	103.72	106.78
13	A	824	CLA	CGD-CBD-CHA	3.75	123.70	110.96
15	J	1104	BCR	C15-C14-C13	-3.74	121.90	127.29
13	B	809	CLA	C1D-C2D-C3D	-3.74	103.72	106.78
13	A	835	CLA	C4D-CHA-CBD	-3.75	100.55	109.37
13	A	812	CLA	O1D-CGD-CBD	-3.74	116.75	124.42
15	B	841	BCR	C2-C1-C6	3.74	116.66	110.44
13	A	807	CLA	C4A-NA-C1A	3.74	111.67	106.52
13	A	810	CLA	C1D-C2D-C3D	-3.73	103.73	106.78
15	A	849	BCR	C15-C14-C13	-3.74	121.91	127.29
15	A	850	BCR	C33-C5-C4	3.73	120.19	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	849	BCR	C7-C8-C9	-3.73	120.63	126.22
13	A	826	CLA	C2D-C1D-ND	3.73	112.23	109.41
13	J	1102	CLA	C2D-C1D-ND	3.73	112.23	109.41
13	A	818	CLA	C2D-C1D-ND	3.73	112.23	109.41
13	A	811	CLA	C1D-C2D-C3D	-3.73	103.73	106.78
13	A	842	CLA	C2D-C1D-ND	3.73	112.23	109.41
13	B	817	CLA	CGD-CBD-CHA	3.73	123.62	110.96
15	A	847	BCR	C33-C5-C4	3.72	120.17	113.34
13	B	816	CLA	C4-C3-C5	3.72	121.05	115.39
13	B	806	CLA	C1D-C2D-C3D	-3.72	103.74	106.78
13	A	825	CLA	C4A-NA-C1A	3.72	111.65	106.52
13	A	809	CLA	O2A-CGA-CBA	3.72	123.64	111.94
15	B	849	BCR	C33-C5-C6	-3.72	120.29	124.51
13	B	803	CLA	C1D-C2D-C3D	-3.72	103.74	106.78
15	L	1006	BCR	C20-C21-C22	-3.72	121.94	127.29
13	B	838	CLA	C2D-C1D-ND	3.72	112.22	109.41
13	A	845	CLA	C1D-C2D-C3D	-3.72	103.74	106.78
13	B	839	CLA	C2D-C1D-ND	3.71	112.21	109.41
15	A	851	BCR	C33-C5-C4	3.71	120.15	113.34
13	B	827	CLA	C1D-C2D-C3D	-3.71	103.75	106.78
13	B	814	CLA	C4A-NA-C1A	3.70	111.63	106.52
13	B	838	CLA	C4-C3-C5	3.70	121.02	115.39
13	A	813	CLA	C2D-C1D-ND	3.70	112.20	109.41
13	L	1003	CLA	C2D-C1D-ND	3.70	112.20	109.41
15	J	1104	BCR	C2-C1-C6	3.70	116.58	110.44
13	A	845	CLA	CAA-CBA-CGA	-3.69	101.36	113.27
13	B	832	CLA	C1D-C2D-C3D	-3.69	103.77	106.78
13	A	812	CLA	CGD-CBD-CHA	3.69	123.49	110.96
13	A	820	CLA	CGD-CBD-CHA	3.68	123.48	110.96
13	A	838	CLA	CGD-CBD-CHA	3.69	123.49	110.96
13	A	803	CLA	O2D-CGD-CBD	3.69	118.84	111.33
15	J	1105	BCR	C24-C23-C22	-3.68	120.71	126.22
13	A	832	CLA	C2D-C1D-ND	3.68	112.19	109.41
13	A	826	CLA	C4A-NA-C1A	3.68	111.59	106.52
13	A	830	CLA	C4-C3-C5	3.68	120.98	115.39
13	B	813	CLA	C2D-C1D-ND	3.68	112.19	109.41
13	F	1301	CLA	C4A-NA-C1A	3.68	111.59	106.52
15	B	845	BCR	C33-C5-C4	3.67	120.08	113.34
13	B	834	CLA	C2D-C1D-ND	3.67	112.18	109.41
13	A	805	CLA	CGD-CBD-CHA	3.66	123.41	110.96
13	B	813	CLA	C1D-C2D-C3D	-3.66	103.79	106.78
13	B	819	CLA	C1D-C2D-C3D	-3.66	103.79	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	816	CLA	C1D-C2D-C3D	-3.66	103.79	106.78
15	M	1203	BCR	C38-C26-C25	-3.66	120.36	124.51
13	B	817	CLA	C2D-C1D-ND	3.65	112.17	109.41
15	B	847	BCR	C20-C21-C22	-3.65	122.03	127.29
15	L	1005	BCR	C2-C1-C6	3.65	116.51	110.44
13	A	845	CLA	C4A-NA-C1A	3.65	111.55	106.52
13	B	837	CLA	C1-O2A-CGA	3.65	119.34	115.06
13	B	824	CLA	C2D-C1D-ND	3.65	112.17	109.41
13	A	855	CLA	CGD-CBD-CHA	3.65	123.36	110.96
13	A	806	CLA	O2D-CGD-CBD	3.65	118.76	111.33
13	B	815	CLA	C1D-C2D-C3D	-3.65	103.80	106.78
15	B	849	BCR	C16-C17-C18	-3.65	122.04	127.29
13	B	802	CLA	C4D-C3D-CAD	-3.64	103.57	108.05
13	A	827	CLA	C1D-C2D-C3D	-3.64	103.80	106.78
13	B	828	CLA	C2D-C1D-ND	3.64	112.16	109.41
13	X	102	CLA	C2D-C1D-ND	3.64	112.16	109.41
13	B	830	CLA	C4A-NA-C1A	3.64	111.54	106.52
13	A	817	CLA	C1D-C2D-C3D	-3.64	103.81	106.78
13	B	824	CLA	CBD-CHA-C1A	3.64	133.52	128.77
15	B	847	BCR	C33-C5-C4	3.64	120.02	113.34
13	A	823	CLA	C4D-CHA-CBD	-3.64	100.81	109.37
15	B	846	BCR	C33-C5-C4	3.63	120.01	113.34
15	F	1302	BCR	C38-C26-C27	3.63	120.01	113.34
13	A	823	CLA	C1-C2-C3	-3.63	119.72	126.19
15	B	845	BCR	C33-C5-C6	-3.63	120.39	124.51
13	B	804	CLA	C1-C2-C3	-3.63	119.73	126.19
13	B	806	CLA	C4A-NA-C1A	3.63	111.52	106.52
13	B	807	CLA	O1D-CGD-CBD	-3.63	116.99	124.42
13	A	821	CLA	C2D-C1D-ND	3.63	112.15	109.41
13	B	833	CLA	C4A-NA-C1A	3.62	111.52	106.52
13	B	810	CLA	C2D-C1D-ND	3.62	112.15	109.41
13	A	855	CLA	C2D-C1D-ND	3.62	112.14	109.41
15	A	850	BCR	C20-C21-C22	-3.62	122.08	127.29
15	M	1203	BCR	C33-C5-C4	3.62	119.98	113.34
13	B	822	CLA	C4A-NA-C1A	3.61	111.50	106.52
13	M	1201	CLA	C4A-NA-C1A	3.61	111.50	106.52
13	B	834	CLA	C1D-C2D-C3D	-3.61	103.83	106.78
13	A	815	CLA	C2D-C1D-ND	3.61	112.14	109.41
13	A	836	CLA	C2D-C1D-ND	3.61	112.13	109.41
15	A	850	BCR	C2-C1-C6	3.60	116.43	110.44
15	A	850	BCR	C16-C17-C18	-3.60	122.10	127.29
13	J	1101	CLA	C2D-C1D-ND	3.60	112.13	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	823	CLA	O2A-CGA-CBA	3.60	121.59	110.52
13	A	821	CLA	C4D-CHA-CBD	-3.60	100.89	109.37
13	A	810	CLA	C4A-NA-C1A	3.60	111.48	106.52
13	A	815	CLA	O1D-CGD-CBD	-3.60	117.05	124.42
13	B	810	CLA	CGD-CBD-CHA	3.60	123.19	110.96
13	B	811	CLA	CGD-CBD-CHA	3.59	123.17	110.96
13	A	834	CLA	C1D-C2D-C3D	-3.59	103.84	106.78
13	M	1202	CLA	C1D-C2D-C3D	-3.59	103.84	106.78
13	B	836	CLA	C2D-C1D-ND	3.59	112.12	109.41
13	A	825	CLA	C1D-C2D-C3D	-3.59	103.85	106.78
13	A	812	CLA	C4A-NA-C1A	3.59	111.47	106.52
15	I	102	BCR	C23-C24-C25	-3.59	116.73	127.32
13	A	809	CLA	CBD-CHA-C1A	3.59	133.46	128.77
13	B	825	CLA	C1D-C2D-C3D	-3.58	103.85	106.78
13	A	843	CLA	C4A-NA-C1A	3.59	111.46	106.52
13	B	839	CLA	C3D-CAD-CBD	-3.58	102.53	107.60
13	A	821	CLA	C1-C2-C3	-3.58	119.81	126.19
13	A	816	CLA	C4A-NA-C1A	3.59	111.46	106.52
13	A	838	CLA	C4A-NA-C1A	3.58	111.46	106.52
15	J	1105	BCR	C16-C17-C18	-3.58	122.13	127.29
13	L	1002	CLA	CGD-CBD-CHA	3.58	123.14	110.96
15	A	848	BCR	C2-C1-C6	3.58	116.39	110.44
13	B	810	CLA	C4A-NA-C1A	3.58	111.46	106.52
13	B	818	CLA	CGD-CBD-CHA	3.58	123.13	110.96
15	F	1302	BCR	C38-C26-C25	-3.58	120.45	124.51
13	A	818	CLA	O2D-CGD-O1D	-3.58	116.52	123.79
13	A	818	CLA	C4-C3-C5	3.58	120.83	115.39
13	A	831	CLA	C4A-NA-C1A	3.57	111.45	106.52
15	M	1203	BCR	C24-C23-C22	-3.57	120.87	126.22
13	A	806	CLA	C2D-C1D-ND	3.57	112.11	109.41
13	B	804	CLA	C4-C3-C5	3.57	120.82	115.39
13	A	835	CLA	C2D-C1D-ND	3.57	112.10	109.41
13	B	836	CLA	C1D-C2D-C3D	-3.57	103.87	106.78
13	A	827	CLA	C4A-NA-C1A	3.56	111.43	106.52
13	B	817	CLA	C4A-NA-C1A	3.56	111.43	106.52
13	B	807	CLA	C4A-NA-C1A	3.56	111.43	106.52
13	A	834	CLA	C4D-CHA-CBD	-3.56	100.99	109.37
13	A	832	CLA	C4A-NA-C1A	3.56	111.42	106.52
15	B	845	BCR	C2-C1-C6	3.55	116.35	110.44
13	A	841	CLA	C2D-C1D-ND	3.55	112.09	109.41
13	B	820	CLA	C4-C3-C5	3.55	120.79	115.39
13	B	818	CLA	C2D-C1D-ND	3.55	112.09	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	825	CLA	C2D-C1D-ND	3.55	112.09	109.41
13	A	818	CLA	C4A-NA-C1A	3.55	111.41	106.52
13	A	840	CLA	CGD-CBD-CHA	3.55	123.02	110.96
15	A	849	BCR	C33-C5-C4	3.55	119.86	113.34
13	A	820	CLA	C1D-C2D-C3D	-3.55	103.88	106.78
13	B	838	CLA	O2A-CGA-CBA	3.55	123.10	111.94
13	L	1004	CLA	C3D-CAD-CBD	-3.55	102.58	107.60
15	A	850	BCR	C11-C10-C9	-3.54	122.19	127.29
13	B	826	CLA	O2D-CGD-CBD	3.54	118.54	111.33
13	A	811	CLA	C4A-NA-C1A	3.54	111.40	106.52
13	A	821	CLA	C4A-NA-C1A	3.54	111.40	106.52
13	A	820	CLA	C4A-NA-C1A	3.54	111.39	106.52
13	X	102	CLA	C1D-C2D-C3D	-3.54	103.89	106.78
13	A	843	CLA	C4-C3-C5	3.54	120.77	115.39
13	B	804	CLA	C1D-C2D-C3D	-3.54	103.89	106.78
13	A	819	CLA	C3D-CAD-CBD	-3.53	102.60	107.60
13	B	831	CLA	C4A-NA-C1A	3.53	111.39	106.52
15	B	845	BCR	C38-C26-C27	3.53	119.82	113.34
13	B	805	CLA	O2D-CGD-CBD	3.53	118.52	111.33
13	A	835	CLA	C3D-CAD-CBD	-3.53	102.61	107.60
13	A	839	CLA	O2D-CGD-O1D	-3.53	116.62	123.79
15	B	846	BCR	C2-C1-C6	3.52	116.30	110.44
15	L	1005	BCR	C16-C15-C14	-3.52	115.56	123.36
13	L	1002	CLA	C1D-C2D-C3D	-3.52	103.90	106.78
13	J	1102	CLA	C1D-C2D-C3D	-3.52	103.90	106.78
13	L	1004	CLA	C2D-C1D-ND	3.52	112.07	109.41
13	A	829	CLA	C2D-C1D-ND	3.52	112.07	109.41
15	I	102	BCR	C33-C5-C4	3.52	119.80	113.34
13	B	805	CLA	C2D-C1D-ND	3.52	112.06	109.41
13	A	818	CLA	C1D-C2D-C3D	-3.51	103.91	106.78
13	A	812	CLA	C1D-C2D-C3D	-3.51	103.91	106.78
15	A	847	BCR	C20-C21-C22	-3.51	122.23	127.29
13	I	101	CLA	C4A-NA-C1A	3.51	111.36	106.52
13	B	808	CLA	C1D-C2D-C3D	-3.51	103.91	106.78
13	B	821	CLA	C1D-C2D-C3D	-3.51	103.91	106.78
13	A	837	CLA	C4A-NA-C1A	3.51	111.36	106.52
15	B	845	BCR	C20-C21-C22	-3.51	122.24	127.29
13	B	838	CLA	C4A-NA-C1A	3.51	111.35	106.52
13	B	832	CLA	C4A-NA-C1A	3.51	111.35	106.52
15	B	846	BCR	C38-C26-C27	3.50	119.76	113.34
13	A	843	CLA	O1D-CGD-CBD	-3.50	117.26	124.42
13	A	824	CLA	C2D-C1D-ND	3.49	112.05	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	1105	BCR	C15-C14-C13	-3.49	122.26	127.29
13	A	833	CLA	C4A-NA-C1A	3.49	111.33	106.52
15	L	1005	BCR	C11-C10-C9	-3.49	122.27	127.29
13	B	805	CLA	C4A-NA-C1A	3.49	111.33	106.52
13	A	819	CLA	C1D-C2D-C3D	-3.49	103.93	106.78
13	B	822	CLA	C1D-C2D-C3D	-3.48	103.93	106.78
13	B	830	CLA	O2D-CGD-O1D	-3.48	116.71	123.79
13	B	834	CLA	C4A-NA-C1A	3.48	111.32	106.52
13	L	1004	CLA	C4A-NA-C1A	3.48	111.32	106.52
13	A	836	CLA	C4D-CHA-CBD	-3.48	101.18	109.37
13	B	829	CLA	CAA-CBA-CGA	-3.48	102.06	113.27
15	I	102	BCR	C16-C17-C18	-3.48	122.28	127.29
15	L	1006	BCR	C2-C1-C6	3.47	116.21	110.44
13	A	805	CLA	C1D-C2D-C3D	-3.47	103.94	106.78
13	A	832	CLA	CGD-CBD-CHA	3.47	122.77	110.96
13	B	820	CLA	C4A-NA-C1A	3.47	111.31	106.52
15	B	841	BCR	C38-C26-C27	3.47	119.71	113.34
13	L	1003	CLA	C4A-NA-C1A	3.47	111.31	106.52
15	J	1105	BCR	C2-C1-C6	3.47	116.21	110.44
13	A	855	CLA	C4A-NA-C1A	3.47	111.31	106.52
13	A	836	CLA	C4A-NA-C1A	3.47	111.30	106.52
13	A	826	CLA	C1D-C2D-C3D	-3.47	103.94	106.78
13	A	813	CLA	C4A-NA-C1A	3.47	111.30	106.52
13	B	822	CLA	C3D-CAD-CBD	-3.47	102.69	107.60
13	A	803	CLA	C1D-C2D-C3D	-3.47	103.95	106.78
13	A	804	CLA	C4A-NA-C1A	3.47	111.30	106.52
13	A	805	CLA	O2A-C1-C2	3.46	116.05	108.55
13	L	1003	CLA	O1D-CGD-CBD	-3.46	117.33	124.42
13	A	806	CLA	C4A-NA-C1A	3.46	111.29	106.52
15	B	850	BCR	C20-C21-C22	-3.46	122.31	127.29
13	B	833	CLA	C2D-C1D-ND	3.46	112.02	109.41
13	B	820	CLA	C1D-C2D-C3D	-3.46	103.95	106.78
15	A	847	BCR	C29-C30-C25	3.45	116.18	110.44
13	B	839	CLA	CGD-CBD-CHA	3.45	122.69	110.96
13	M	1201	CLA	O1D-CGD-CBD	-3.45	117.35	124.42
15	B	842	BCR	C38-C26-C27	3.45	119.67	113.34
13	B	837	CLA	C4A-NA-C1A	3.45	111.27	106.52
13	B	828	CLA	C1D-C2D-C3D	-3.45	103.96	106.78
13	A	832	CLA	C1D-C2D-C3D	-3.45	103.97	106.78
13	B	826	CLA	C4A-NA-C1A	3.45	111.27	106.52
13	A	805	CLA	C4A-NA-C1A	3.44	111.27	106.52
15	A	850	BCR	C33-C5-C6	-3.44	120.61	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	817	CLA	O2D-CGD-O1D	-3.44	116.80	123.79
13	B	823	CLA	C1D-C2D-C3D	-3.44	103.97	106.78
13	B	837	CLA	C1D-C2D-C3D	-3.44	103.97	106.78
13	J	1102	CLA	C4A-NA-C1A	3.44	111.26	106.52
13	A	843	CLA	C1D-C2D-C3D	-3.44	103.97	106.78
13	B	839	CLA	C4A-NA-C1A	3.44	111.26	106.52
13	B	804	CLA	C4A-NA-C1A	3.44	111.26	106.52
13	A	823	CLA	C4A-NA-C1A	3.43	111.25	106.52
13	J	1103	CLA	C2D-C1D-ND	3.43	112.00	109.41
13	B	836	CLA	C3D-CAD-CBD	-3.43	102.75	107.60
13	L	1002	CLA	C4A-NA-C1A	3.43	111.25	106.52
13	B	809	CLA	C4A-NA-C1A	3.43	111.25	106.52
13	B	819	CLA	C4A-NA-C1A	3.43	111.25	106.52
13	B	823	CLA	CAA-C2A-C1A	3.43	120.17	111.62
13	B	825	CLA	C4-C3-C5	3.42	120.59	115.39
13	B	839	CLA	C1D-C2D-C3D	-3.42	103.98	106.78
13	A	803	CLA	C4A-NA-C1A	3.42	111.24	106.52
15	A	847	BCR	C38-C26-C27	3.42	119.62	113.34
13	B	804	CLA	CGD-CBD-CHA	3.42	122.59	110.96
13	A	825	CLA	O1D-CGD-CBD	-3.42	117.41	124.42
15	B	850	BCR	C33-C5-C6	-3.42	120.63	124.51
13	A	829	CLA	C4A-NA-C1A	3.41	111.23	106.52
13	A	837	CLA	CAA-C2A-C1A	3.41	120.14	111.62
13	B	815	CLA	C4A-NA-C1A	3.41	111.23	106.52
15	B	841	BCR	C20-C21-C22	-3.41	122.38	127.29
13	B	811	CLA	C2D-C1D-ND	3.41	111.99	109.41
13	B	835	CLA	C4A-NA-C1A	3.41	111.22	106.52
13	J	1101	CLA	C4A-NA-C1A	3.41	111.22	106.52
13	A	835	CLA	C4A-NA-C1A	3.41	111.22	106.52
13	A	841	CLA	C4A-NA-C1A	3.41	111.22	106.52
13	A	817	CLA	C4A-NA-C1A	3.41	111.22	106.52
13	A	821	CLA	O2D-CGD-O1D	-3.41	116.87	123.79
13	A	813	CLA	C1D-C2D-C3D	-3.40	104.00	106.78
13	A	829	CLA	C1D-C2D-C3D	-3.40	104.00	106.78
15	F	1302	BCR	C20-C21-C22	-3.40	122.39	127.29
13	B	805	CLA	C4D-CHA-CBD	-3.40	101.36	109.37
13	A	828	CLA	C4A-NA-C1A	3.40	111.21	106.52
13	A	828	CLA	C4-C3-C5	3.40	120.55	115.39
13	B	827	CLA	C2C-C1C-NC	-3.40	107.42	110.17
13	B	818	CLA	C4A-NA-C1A	3.40	111.20	106.52
13	B	811	CLA	C1D-C2D-C3D	-3.39	104.01	106.78
13	A	840	CLA	C4A-NA-C1A	3.39	111.20	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	819	CLA	CBA-CAA-C2A	-3.39	103.95	114.01
15	B	843	BCR	C23-C22-C21	-3.39	113.77	118.97
13	B	825	CLA	C4A-NA-C1A	3.38	111.18	106.52
13	B	821	CLA	C4A-NA-C1A	3.38	111.18	106.52
13	B	823	CLA	C4A-NA-C1A	3.38	111.18	106.52
13	B	836	CLA	C4A-NA-C1A	3.38	111.18	106.52
13	A	802	CLA	C1-C2-C3	-3.38	120.17	126.19
16	X	101	LHG	O7-C7-C8	3.38	118.97	111.56
13	A	823	CLA	CGD-CBD-CHA	3.38	122.45	110.96
13	A	855	CLA	C1D-C2D-C3D	-3.38	104.02	106.78
13	A	815	CLA	C4A-NA-C1A	3.38	111.18	106.52
13	B	829	CLA	C1D-C2D-C3D	-3.38	104.02	106.78
15	B	846	BCR	C24-C23-C22	-3.38	121.17	126.22
13	A	812	CLA	C4-C3-C5	3.38	120.52	115.39
13	A	841	CLA	CGD-CBD-CHA	3.38	122.43	110.96
13	B	811	CLA	O2A-CGA-CBA	3.37	122.55	111.94
13	A	822	CLA	C4A-NA-C1A	3.37	111.17	106.52
13	A	842	CLA	C4A-NA-C1A	3.37	111.17	106.52
15	M	1203	BCR	C16-C17-C18	-3.37	122.43	127.29
13	A	804	CLA	C4-C3-C5	3.37	120.51	115.39
13	B	811	CLA	C4A-NA-C1A	3.37	111.17	106.52
13	B	829	CLA	O2D-CGD-CBD	3.37	118.19	111.33
13	B	825	CLA	C3D-CAD-CBD	-3.37	102.83	107.60
13	B	808	CLA	C4A-NA-C1A	3.37	111.16	106.52
13	A	828	CLA	C1-C2-C3	-3.37	120.20	126.19
13	B	808	CLA	C4-C3-C5	3.36	120.50	115.39
15	F	1302	BCR	C7-C8-C9	-3.36	121.18	126.22
13	B	828	CLA	C3B-CAB-CBB	-3.36	118.99	125.95
13	A	808	CLA	O2A-CGA-CBA	3.36	122.50	111.94
13	B	803	CLA	C4-C3-C5	3.36	120.49	115.39
13	A	839	CLA	C4D-CHA-CBD	-3.36	101.47	109.37
13	A	842	CLA	C1D-C2D-C3D	-3.36	104.04	106.78
13	B	812	CLA	C4-C3-C5	3.35	120.49	115.39
13	B	817	CLA	C4-C3-C5	3.35	120.48	115.39
13	B	824	CLA	C4-C3-C5	3.35	120.49	115.39
13	B	822	CLA	C2D-C1D-ND	3.35	111.94	109.41
13	B	816	CLA	C4A-NA-C1A	3.35	111.14	106.52
15	F	1302	BCR	C2-C1-C6	3.35	116.01	110.44
13	B	816	CLA	CGD-CBD-CHA	3.35	122.33	110.96
13	A	841	CLA	O2D-CGD-CBD	3.34	118.14	111.33
13	A	831	CLA	CGD-CBD-CHA	3.34	122.32	110.96
13	B	823	CLA	C3D-CAD-CBD	-3.34	102.88	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	834	CLA	C4-C3-C5	3.34	120.46	115.39
13	B	824	CLA	C1D-C2D-C3D	-3.34	104.05	106.78
13	A	841	CLA	C1D-C2D-C3D	-3.34	104.06	106.78
13	B	812	CLA	C4A-NA-C1A	3.33	111.11	106.52
13	B	829	CLA	C4A-NA-C1A	3.33	111.11	106.52
13	J	1101	CLA	C1D-C2D-C3D	-3.33	104.06	106.78
13	B	823	CLA	C2D-C1D-ND	3.33	111.92	109.41
13	A	812	CLA	C1-C2-C3	-3.33	120.26	126.19
13	A	824	CLA	C1D-C2D-C3D	-3.33	104.06	106.78
13	A	814	CLA	C4A-NA-C1A	3.33	111.11	106.52
13	A	824	CLA	O1D-CGD-CBD	-3.33	117.61	124.42
14	A	846	PQN	C11-C12-C13	-3.33	121.14	126.76
13	A	806	CLA	C1D-C2D-C3D	-3.32	104.06	106.78
15	A	847	BCR	C24-C23-C22	-3.32	121.24	126.22
13	L	1004	CLA	C1D-C2D-C3D	-3.32	104.06	106.78
13	A	833	CLA	C3D-CAD-CBD	-3.32	102.90	107.60
13	B	824	CLA	C4A-NA-C1A	3.32	111.10	106.52
13	I	101	CLA	C4-C3-C5	3.32	120.44	115.39
13	A	827	CLA	CGD-CBD-CHA	3.32	122.23	110.96
13	J	1101	CLA	CBD-CHA-C1A	3.31	133.10	128.77
13	A	821	CLA	C1D-C2D-C3D	-3.31	104.08	106.78
15	B	845	BCR	C15-C16-C17	-3.31	116.03	123.36
13	B	805	CLA	C1D-C2D-C3D	-3.31	104.08	106.78
13	A	839	CLA	C1D-C2D-C3D	-3.31	104.08	106.78
13	A	816	CLA	C1D-C2D-C3D	-3.31	104.08	106.78
15	I	102	BCR	C15-C14-C13	-3.31	122.53	127.29
15	B	841	BCR	C29-C30-C25	3.31	115.93	110.44
13	B	801	CLA	C1D-C2D-C3D	-3.30	104.08	106.78
13	A	832	CLA	C4-C3-C5	3.30	120.41	115.39
13	B	802	CLA	C3B-CAB-CBB	-3.30	119.11	125.95
13	X	102	CLA	C4A-NA-C1A	3.30	111.07	106.52
15	F	1302	BCR	C24-C23-C22	-3.29	121.29	126.22
13	B	837	CLA	O1D-CGD-CBD	-3.29	117.68	124.42
15	J	1105	BCR	C29-C30-C25	3.28	115.90	110.44
15	B	847	BCR	C12-C13-C14	-3.28	113.92	118.97
15	B	849	BCR	C15-C16-C17	-3.28	116.09	123.36
13	B	817	CLA	C1D-C2D-C3D	-3.28	104.10	106.78
15	B	841	BCR	C24-C23-C22	-3.28	121.31	126.22
15	F	1302	BCR	C15-C16-C17	-3.28	116.10	123.36
15	J	1104	BCR	C16-C17-C18	-3.28	122.57	127.29
13	B	839	CLA	C4-C3-C5	3.28	120.37	115.39
13	B	801	CLA	C1-C2-C3	-3.28	120.36	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	803	CLA	C4-C3-C5	3.28	120.37	115.39
13	A	809	CLA	C4-C3-C5	3.28	120.37	115.39
13	A	806	CLA	CGD-CBD-CHA	3.27	122.08	110.96
13	B	827	CLA	C4-C3-C5	3.27	120.36	115.39
13	B	826	CLA	C1D-C2D-C3D	-3.27	104.11	106.78
15	B	849	BCR	C23-C24-C25	-3.27	117.66	127.32
15	B	846	BCR	C10-C11-C12	-3.27	112.22	123.24
13	A	811	CLA	C4-C3-C5	3.27	120.36	115.39
13	L	1003	CLA	C1-C2-C3	-3.26	120.38	126.19
13	B	812	CLA	C1D-C2D-C3D	-3.26	104.11	106.78
15	M	1203	BCR	C10-C11-C12	-3.26	112.23	123.24
13	A	823	CLA	C3D-CAD-CBD	-3.26	102.99	107.60
13	L	1004	CLA	C4-C3-C5	3.26	120.34	115.39
13	A	824	CLA	C4-C3-C5	3.26	120.34	115.39
13	B	828	CLA	C4A-NA-C1A	3.26	111.01	106.52
13	A	822	CLA	CGD-CBD-CHA	3.25	122.02	110.96
15	A	848	BCR	C20-C21-C22	-3.25	122.61	127.29
13	A	836	CLA	CGD-CBD-CHA	3.25	122.01	110.96
13	B	812	CLA	C2D-C1D-ND	3.25	111.86	109.41
15	A	852	BCR	C29-C30-C25	3.25	115.84	110.44
15	A	851	BCR	C20-C21-C22	-3.25	122.61	127.29
13	B	838	CLA	C1D-C2D-C3D	-3.25	104.12	106.78
13	A	803	CLA	CGD-CBD-CHA	3.25	122.00	110.96
13	B	830	CLA	C1D-C2D-C3D	-3.25	104.13	106.78
15	A	851	BCR	C2-C1-C6	3.24	115.83	110.44
13	A	814	CLA	CGD-CBD-CHA	3.24	121.97	110.96
13	B	818	CLA	C1D-C2D-C3D	-3.24	104.13	106.78
13	L	1003	CLA	C1D-C2D-C3D	-3.24	104.13	106.78
13	A	811	CLA	O1D-CGD-CBD	-3.24	117.79	124.42
13	A	834	CLA	C4A-NA-C1A	3.24	110.98	106.52
13	B	807	CLA	C1-C2-C3	-3.23	120.44	126.19
13	F	1301	CLA	O2D-CGD-O1D	-3.23	117.22	123.79
13	A	803	CLA	C1-C2-C3	-3.23	120.44	126.19
15	B	846	BCR	C29-C30-C25	3.23	115.81	110.44
13	A	815	CLA	C1D-C2D-C3D	-3.22	104.15	106.78
15	B	850	BCR	C23-C24-C25	-3.22	117.80	127.32
13	A	827	CLA	C4-C3-C5	3.22	120.29	115.39
13	A	843	CLA	CGD-CBD-CHA	3.22	121.92	110.96
15	A	849	BCR	C2-C1-C6	3.22	115.79	110.44
13	A	829	CLA	C4-C3-C5	3.22	120.28	115.39
13	A	805	CLA	C3D-CAD-CBD	-3.22	103.05	107.60
13	A	802	CLA	C1D-C2D-C3D	-3.22	104.15	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	830	CLA	C4D-CHA-CBD	-3.21	101.80	109.37
15	B	842	BCR	C33-C5-C4	3.21	119.23	113.34
15	B	847	BCR	C24-C23-C22	-3.21	121.41	126.22
13	A	820	CLA	C1-C2-C3	-3.21	120.48	126.19
13	A	835	CLA	C4-C3-C5	3.21	120.27	115.39
13	B	806	CLA	CGD-CBD-CHA	3.20	121.85	110.96
13	B	806	CLA	C4-C3-C5	3.20	120.26	115.39
13	A	838	CLA	C4-C3-C5	3.20	120.25	115.39
13	A	807	CLA	C3D-CAD-CBD	-3.20	103.08	107.60
13	A	802	CLA	C2D-C1D-ND	3.20	111.82	109.41
13	B	804	CLA	C3D-CAD-CBD	-3.19	103.08	107.60
15	B	841	BCR	C15-C14-C13	-3.19	122.70	127.29
13	B	833	CLA	C1D-C2D-C3D	-3.19	104.17	106.78
13	A	833	CLA	O2D-CGD-CBD	3.19	117.83	111.33
13	A	823	CLA	O2D-CGD-CBD	3.19	117.82	111.33
13	B	817	CLA	C4D-CHA-CBD	-3.18	101.88	109.37
13	L	1003	CLA	CAA-C2A-C3A	-3.18	105.52	113.04
13	B	801	CLA	O1D-CGD-CBD	-3.18	117.90	124.42
13	A	844	CLA	C2D-C1D-ND	3.18	111.81	109.41
13	B	813	CLA	O1D-CGD-CBD	-3.17	117.92	124.42
13	I	101	CLA	C1-C2-C3	-3.17	120.55	126.19
13	A	806	CLA	C4-C3-C5	3.16	120.20	115.39
13	A	813	CLA	C4-C3-C5	3.16	120.19	115.39
13	A	822	CLA	C3B-CAB-CBB	-3.16	119.41	125.95
13	B	838	CLA	C3B-CAB-CBB	-3.16	119.41	125.95
15	B	843	BCR	C33-C5-C4	3.15	119.13	113.34
15	M	1203	BCR	C15-C14-C13	-3.15	122.75	127.29
13	B	810	CLA	C1D-C2D-C3D	-3.15	104.20	106.78
13	B	803	CLA	C4D-C3D-CAD	-3.15	104.18	108.05
15	B	843	BCR	C7-C8-C9	-3.15	121.50	126.22
13	B	830	CLA	C4-C3-C5	3.15	120.18	115.39
13	B	838	CLA	C1-C2-C3	-3.14	120.60	126.19
13	B	831	CLA	O2D-CGD-O1D	-3.14	117.41	123.79
15	B	843	BCR	C10-C11-C12	-3.14	112.64	123.24
13	B	826	CLA	C3D-CAD-CBD	-3.14	103.16	107.60
15	I	102	BCR	C24-C23-C22	-3.14	121.52	126.22
13	B	807	CLA	C3D-CAD-CBD	-3.13	103.17	107.60
13	A	832	CLA	O2A-CGA-CBA	3.13	121.80	111.94
15	A	850	BCR	C29-C30-C25	3.13	115.64	110.44
13	B	817	CLA	O1D-CGD-CBD	-3.13	118.00	124.42
13	B	807	CLA	C4-C3-C5	3.13	120.15	115.39
13	B	802	CLA	C4-C3-C5	3.13	120.15	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	815	CLA	C4-C3-C5	3.13	120.15	115.39
15	B	844	BCR	C29-C30-C25	3.13	115.64	110.44
13	A	818	CLA	C3D-CAD-CBD	-3.13	103.18	107.60
13	A	829	CLA	O1D-CGD-CBD	-3.13	118.02	124.42
15	A	848	BCR	C29-C30-C25	3.13	115.63	110.44
15	M	1203	BCR	C29-C30-C25	3.12	115.63	110.44
13	B	801	CLA	C4-C3-C5	3.12	120.13	115.39
15	B	847	BCR	C8-C7-C6	-3.12	118.11	127.32
15	M	1203	BCR	C20-C21-C22	-3.12	122.80	127.29
13	B	810	CLA	O2D-CGD-CBD	3.12	117.68	111.33
15	I	102	BCR	C8-C7-C6	-3.11	118.13	127.32
15	J	1105	BCR	C20-C21-C22	-3.11	122.81	127.29
13	B	820	CLA	C1-C2-C3	-3.11	120.66	126.19
13	B	822	CLA	C4-C3-C5	3.11	120.12	115.39
13	A	824	CLA	C4A-NA-C1A	3.11	110.81	106.52
13	L	1002	CLA	C4-C3-C5	3.11	120.12	115.39
15	A	849	BCR	C29-C30-C25	3.11	115.60	110.44
13	B	813	CLA	C4A-NA-C1A	3.10	110.80	106.52
13	A	836	CLA	C1D-C2D-C3D	-3.10	104.25	106.78
15	A	851	BCR	C7-C8-C9	-3.10	121.58	126.22
13	A	817	CLA	C1-C2-C3	-3.10	120.68	126.19
13	A	810	CLA	O1D-CGD-CBD	-3.09	118.08	124.42
13	A	801	CLA	C4-C3-C5	3.09	120.09	115.39
13	B	833	CLA	O2D-CGD-O1D	-3.09	117.51	123.79
13	J	1102	CLA	CBD-CHA-C1A	3.09	132.80	128.77
13	A	807	CLA	C4-C3-C5	3.09	121.82	114.77
13	A	806	CLA	C3D-CAD-CBD	-3.08	103.24	107.60
13	A	802	CLA	C4-C3-C5	3.08	120.08	115.39
13	B	808	CLA	O1D-CGD-CBD	-3.08	118.11	124.42
13	B	830	CLA	CGD-CBD-CHA	3.08	121.44	110.96
15	L	1006	BCR	C29-C30-C25	3.08	115.56	110.44
15	A	852	BCR	C2-C1-C6	3.08	115.56	110.44
13	B	821	CLA	CED-O2D-CGD	3.08	123.34	116.02
13	B	802	CLA	C4A-NA-C1A	3.08	110.76	106.52
13	B	805	CLA	C4-C3-C5	3.08	120.07	115.39
15	B	841	BCR	C10-C11-C12	-3.07	112.87	123.24
13	X	102	CLA	CBD-CHA-C1A	3.07	132.79	128.77
15	A	852	BCR	C7-C8-C9	-3.07	121.62	126.22
13	B	803	CLA	C4A-NA-C1A	3.07	110.75	106.52
13	A	833	CLA	C4-C3-C5	3.07	120.06	115.39
13	A	835	CLA	C1D-C2D-C3D	-3.07	104.27	106.78
13	A	808	CLA	CGD-CBD-CAD	-3.07	100.54	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	820	CLA	C3D-CAD-CBD	-3.06	103.27	107.60
13	A	827	CLA	C2C-C1C-NC	-3.06	107.69	110.17
13	A	837	CLA	C2A-C1A-CHA	3.06	129.14	123.83
13	B	830	CLA	O2A-CGA-CBA	3.06	121.58	111.94
15	B	849	BCR	C2-C1-C6	3.06	115.53	110.44
15	B	846	BCR	C8-C7-C6	-3.06	118.28	127.32
13	B	811	CLA	O1D-CGD-CBD	-3.06	118.15	124.42
15	B	846	BCR	C12-C13-C14	-3.06	114.27	118.97
13	B	805	CLA	CGD-CBD-CHA	3.06	121.35	110.96
13	A	829	CLA	C3B-CAB-CBB	-3.05	119.63	125.95
15	J	1105	BCR	C8-C7-C6	-3.05	118.31	127.32
15	A	849	BCR	C10-C11-C12	-3.05	112.95	123.24
15	A	849	BCR	C23-C24-C25	-3.05	118.32	127.32
13	B	822	CLA	O1D-CGD-CBD	-3.05	118.17	124.42
13	A	809	CLA	CAA-CBA-CGA	-3.05	103.43	113.27
13	M	1201	CLA	C4-C3-C5	3.05	120.02	115.39
15	I	102	BCR	C10-C11-C12	-3.05	112.95	123.24
15	J	1105	BCR	C7-C8-C9	-3.05	121.66	126.22
13	A	802	CLA	C4A-NA-C1A	3.04	110.72	106.52
13	J	1101	CLA	C4-C3-C5	3.04	120.02	115.39
13	A	845	CLA	C3B-CAB-CBB	-3.04	119.65	125.95
15	B	846	BCR	C38-C26-C25	-3.04	121.06	124.51
13	A	845	CLA	C4-C3-C5	3.04	120.01	115.39
15	I	102	BCR	C12-C13-C14	-3.04	114.30	118.97
13	B	824	CLA	O1D-CGD-CBD	-3.04	118.20	124.42
15	B	844	BCR	C24-C23-C22	-3.04	121.67	126.22
13	A	807	CLA	O2A-CGA-CBA	3.03	121.48	111.94
15	L	1005	BCR	C29-C30-C25	3.03	115.48	110.44
13	A	817	CLA	CAA-CBA-CGA	-3.03	103.50	113.27
13	A	824	CLA	C4D-C3D-CAD	-3.02	104.34	108.05
15	A	850	BCR	C15-C14-C13	-3.02	122.94	127.29
13	L	1003	CLA	C4-C3-C5	3.02	119.98	115.39
13	B	820	CLA	O2D-CGD-CBD	3.02	117.48	111.33
13	B	836	CLA	O1D-CGD-CBD	-3.02	118.24	124.42
13	A	828	CLA	O1D-CGD-CBD	-3.02	118.24	124.42
13	A	803	CLA	CBD-CHA-C1A	3.01	132.71	128.77
13	J	1103	CLA	C4A-NA-C1A	3.02	110.68	106.52
13	B	820	CLA	CAA-C2A-C3A	3.01	120.16	113.04
13	B	804	CLA	O2A-CGA-CBA	3.01	121.42	111.94
13	B	827	CLA	O2D-CGD-O1D	-3.01	117.67	123.79
13	A	818	CLA	C5-C6-C7	-3.01	107.60	113.25
13	A	816	CLA	O2D-CGD-CBD	3.01	117.46	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	837	CLA	CAA-C2A-C3A	-3.01	105.93	113.04
13	A	820	CLA	C4-C3-C5	3.00	119.96	115.39
13	B	833	CLA	O1D-CGD-CBD	-3.00	118.27	124.42
13	A	817	CLA	C4-C3-C5	3.00	119.95	115.39
13	A	807	CLA	C3B-CAB-CBB	-3.00	119.74	125.95
13	L	1002	CLA	C4D-C3D-CAD	-3.00	104.36	108.05
13	L	1004	CLA	O2A-CGA-CBA	2.99	121.36	111.94
13	A	801	CLA	O1D-CGD-CBD	-2.99	118.29	124.42
13	A	809	CLA	C1-C2-C3	-2.99	120.86	126.19
13	A	831	CLA	C1-C2-C3	-2.99	120.86	126.19
13	A	817	CLA	O2D-CGD-CBD	2.99	117.42	111.33
15	A	847	BCR	C10-C11-C12	-2.99	113.16	123.24
13	B	811	CLA	CBD-CHA-C1A	2.99	132.68	128.77
13	B	836	CLA	C3B-CAB-CBB	-2.99	119.77	125.95
13	A	816	CLA	O2A-CGA-CBA	2.98	121.33	111.94
13	B	818	CLA	C3B-CAB-CBB	-2.98	119.77	125.95
13	B	831	CLA	C1-C2-C3	-2.98	120.88	126.19
13	M	1201	CLA	C3B-CAB-CBB	-2.98	119.78	125.95
13	A	819	CLA	C5-C3-C2	-2.98	115.35	121.08
13	J	1102	CLA	O1D-CGD-CBD	-2.98	118.33	124.42
13	A	855	CLA	O1D-CGD-CBD	-2.98	118.32	124.42
15	B	843	BCR	C15-C14-C13	-2.97	123.01	127.29
15	B	845	BCR	C10-C11-C12	-2.98	113.20	123.24
15	L	1005	BCR	C20-C21-C22	-2.97	123.01	127.29
13	B	836	CLA	C4-C3-C5	2.97	119.91	115.39
13	B	834	CLA	O1D-CGD-CBD	-2.97	118.33	124.42
13	B	835	CLA	O2A-CGA-CBA	2.97	121.29	111.94
13	A	801	CLA	C4A-NA-C1A	2.97	110.62	106.52
13	A	825	CLA	CGD-CBD-CHA	2.97	121.05	110.96
13	B	813	CLA	C3B-CAB-CBB	-2.97	119.81	125.95
13	A	844	CLA	C3B-CAB-CBB	-2.97	119.81	125.95
13	M	1202	CLA	O1D-CGD-CBD	-2.97	118.35	124.42
13	B	819	CLA	O1D-CGD-CBD	-2.97	118.34	124.42
15	F	1302	BCR	C23-C24-C25	-2.96	118.56	127.32
13	B	832	CLA	O1D-CGD-CBD	-2.96	118.35	124.42
15	B	847	BCR	C7-C8-C9	-2.96	121.79	126.22
15	B	842	BCR	C15-C16-C17	-2.96	116.82	123.36
13	A	824	CLA	O2D-CGD-O1D	-2.96	117.78	123.79
13	B	818	CLA	O2D-CGD-CBD	2.95	117.34	111.33
13	B	809	CLA	O2D-CGD-O1D	-2.95	117.80	123.79
13	B	825	CLA	C1-O2A-CGA	2.95	125.23	116.98
13	B	802	CLA	O2A-CGA-CBA	2.95	121.21	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	823	CLA	C3B-CAB-CBB	-2.94	119.86	125.95
13	A	814	CLA	C3B-CAB-CBB	-2.94	119.86	125.95
13	B	801	CLA	C4A-NA-C1A	2.94	110.58	106.52
13	J	1101	CLA	O2A-CGA-CBA	2.94	121.19	111.94
13	L	1003	CLA	C3B-CAB-CBB	-2.94	119.87	125.95
15	A	847	BCR	C7-C8-C9	-2.94	121.82	126.22
15	L	1006	BCR	C8-C7-C6	-2.94	118.65	127.32
13	A	826	CLA	C3B-CAB-CBB	-2.93	119.88	125.95
13	L	1002	CLA	O1D-CGD-CBD	-2.93	118.41	124.42
13	B	812	CLA	C3B-CAB-CBB	-2.93	119.88	125.95
13	A	824	CLA	C1-C2-C3	-2.93	120.98	126.19
13	L	1002	CLA	C1-C2-C3	-2.93	120.98	126.19
13	B	806	CLA	C1-O2A-CGA	2.93	125.18	116.98
15	J	1104	BCR	C20-C21-C22	-2.93	123.08	127.29
13	B	808	CLA	CBD-CHA-C1A	2.93	132.59	128.77
13	A	813	CLA	O1D-CGD-CBD	-2.93	118.43	124.42
15	F	1302	BCR	C29-C30-C25	2.92	115.30	110.44
13	A	845	CLA	C1-C2-C3	-2.92	121.00	126.19
15	B	842	BCR	C29-C30-C25	2.92	115.29	110.44
13	A	845	CLA	CBD-CHA-C1A	2.91	132.58	128.77
13	B	822	CLA	CBD-CHA-C1A	2.91	132.58	128.77
15	B	841	BCR	C7-C8-C9	-2.91	121.86	126.22
13	B	829	CLA	C3B-CAB-CBB	-2.91	119.92	125.95
18	B	848	LMG	O8-C28-C29	2.91	121.10	111.94
13	F	1301	CLA	C3B-CAB-CBB	-2.91	119.92	125.95
13	A	855	CLA	C3B-CAB-CBB	-2.91	119.93	125.95
13	B	815	CLA	O2D-CGD-CBD	2.91	117.25	111.33
13	A	844	CLA	C4A-NA-C1A	2.90	110.53	106.52
13	A	827	CLA	CBD-CHA-C1A	2.90	132.56	128.77
13	B	814	CLA	O1D-CGD-CBD	-2.90	118.48	124.42
13	A	836	CLA	C3B-CAB-CBB	-2.90	119.95	125.95
13	A	807	CLA	C1-C2-C3	-2.90	121.03	126.19
13	J	1103	CLA	C3B-CAB-CBB	-2.90	119.95	125.95
13	A	826	CLA	C4-C3-C5	2.89	119.78	115.39
15	B	843	BCR	C38-C26-C27	2.89	118.64	113.34
13	A	827	CLA	O2A-CGA-CBA	2.89	121.02	111.94
13	A	837	CLA	O1D-CGD-CBD	-2.89	118.51	124.42
15	B	845	BCR	C8-C7-C6	-2.89	118.80	127.32
15	B	849	BCR	C11-C12-C13	-2.88	118.15	126.38
15	B	841	BCR	C27-C26-C25	-2.88	119.00	122.84
13	B	808	CLA	O2D-CGD-O1D	-2.88	117.94	123.79
13	A	838	CLA	O1D-CGD-CBD	-2.88	118.52	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	815	CLA	C3B-CAB-CBB	-2.88	119.99	125.95
15	J	1104	BCR	C38-C26-C27	2.88	118.62	113.34
13	A	801	CLA	O2D-CGD-O1D	-2.88	117.94	123.79
13	B	826	CLA	C3B-CAB-CBB	-2.88	119.99	125.95
13	A	811	CLA	O2D-CGD-O1D	-2.88	117.95	123.79
15	B	847	BCR	C29-C30-C25	2.88	115.22	110.44
13	A	808	CLA	C1-C2-C3	-2.87	121.08	126.19
13	A	809	CLA	C3A-C2A-C1A	2.87	105.14	101.08
13	B	827	CLA	O1D-CGD-CBD	-2.87	118.54	124.42
13	B	813	CLA	O2D-CGD-O1D	-2.87	117.97	123.79
15	B	844	BCR	C15-C16-C17	-2.87	117.02	123.36
13	B	818	CLA	O2A-CGA-CBA	2.87	120.96	111.94
13	A	838	CLA	OBD-CAD-C3D	-2.86	122.59	127.91
13	B	839	CLA	C3B-CAB-CBB	-2.86	120.04	125.95
13	B	822	CLA	O2D-CGD-O1D	-2.86	117.99	123.79
13	B	812	CLA	C4D-C3D-CAD	-2.85	104.55	108.05
13	B	835	CLA	CAA-C2A-C1A	2.85	118.74	111.62
15	B	842	BCR	C7-C8-C9	-2.85	121.95	126.22
13	J	1103	CLA	C1D-C2D-C3D	-2.84	104.46	106.78
13	A	815	CLA	C2C-C1C-NC	-2.84	107.87	110.17
15	B	841	BCR	C38-C26-C25	-2.84	121.29	124.51
15	A	847	BCR	C38-C26-C25	-2.84	121.29	124.51
13	A	802	CLA	C3B-CAB-CBB	-2.84	120.08	125.95
13	B	814	CLA	O2D-CGD-O1D	-2.83	118.03	123.79
13	A	829	CLA	O2A-C1-C2	-2.83	102.41	108.55
13	B	807	CLA	CMD-C2D-C3D	2.83	129.43	124.97
15	I	102	BCR	C20-C21-C22	-2.83	123.21	127.29
13	B	822	CLA	C1-C2-C3	-2.83	121.16	126.19
13	B	835	CLA	C4-C3-C5	2.83	119.69	115.39
13	L	1003	CLA	CAA-CBA-CGA	-2.83	104.15	113.27
13	B	818	CLA	CBD-CHA-C1A	2.83	132.47	128.77
13	A	801	CLA	C3B-CAB-CBB	-2.83	120.10	125.95
15	J	1105	BCR	C11-C10-C9	-2.83	123.22	127.29
15	A	847	BCR	C27-C26-C25	-2.82	119.09	122.84
15	I	102	BCR	C21-C20-C19	-2.82	113.73	123.24
13	A	807	CLA	CGD-CBD-CAD	-2.82	101.39	110.96
13	L	1004	CLA	C3B-CAB-CBB	-2.82	120.12	125.95
13	B	831	CLA	C4-C3-C5	2.81	119.67	115.39
13	A	818	CLA	C3B-CAB-CBB	-2.81	120.13	125.95
15	L	1006	BCR	C36-C18-C17	-2.81	118.93	122.92
13	B	805	CLA	C1D-CHD-C4C	2.81	126.96	122.60
15	A	849	BCR	C8-C7-C6	-2.81	119.02	127.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	844	BCR	C35-C13-C14	-2.81	119.92	123.91
13	L	1004	CLA	O2D-CGD-O1D	-2.81	118.09	123.79
15	B	844	BCR	C23-C24-C25	-2.81	119.03	127.32
13	B	808	CLA	O2A-CGA-CBA	2.81	120.77	111.94
13	A	837	CLA	O2A-CGA-CBA	2.81	120.77	111.94
13	A	824	CLA	C3B-CAB-CBB	-2.80	120.15	125.95
13	B	811	CLA	C1-C2-C3	-2.80	121.20	126.19
13	A	806	CLA	C3B-CAB-CBB	-2.80	120.16	125.95
13	B	808	CLA	C4D-C3D-CAD	-2.80	104.61	108.05
13	A	820	CLA	C3B-CAB-CBB	-2.80	120.16	125.95
13	A	834	CLA	O1D-CGD-CBD	-2.79	118.70	124.42
13	A	821	CLA	O1D-CGD-CBD	-2.79	118.70	124.42
13	A	845	CLA	O1D-CGD-CBD	-2.79	118.70	124.42
13	A	801	CLA	C1-C2-C3	-2.79	121.23	126.19
13	A	815	CLA	CGD-CBD-CHA	2.78	120.42	110.96
15	I	102	BCR	C11-C10-C9	-2.78	123.28	127.29
13	A	810	CLA	O2D-CGD-O1D	-2.78	118.14	123.79
13	A	805	CLA	O2A-CGA-CBA	2.78	120.67	111.94
13	B	803	CLA	O1D-CGD-CBD	-2.78	118.73	124.42
13	B	808	CLA	CMD-C2D-C3D	2.77	129.34	124.97
13	B	809	CLA	O1D-CGD-CBD	-2.77	118.74	124.42
13	A	841	CLA	O2A-CGA-CBA	2.77	120.66	111.94
15	B	850	BCR	C33-C5-C4	2.77	118.42	113.34
15	M	1203	BCR	C27-C26-C25	-2.77	119.15	122.84
15	L	1005	BCR	C35-C13-C12	2.76	122.56	118.09
13	A	831	CLA	C3B-CAB-CBB	-2.76	120.23	125.95
13	J	1101	CLA	C1-C2-C3	-2.76	121.28	126.19
13	B	831	CLA	C4D-C3D-CAD	-2.75	104.67	108.05
13	B	815	CLA	C3D-CAD-CBD	-2.75	103.70	107.60
13	B	804	CLA	O1D-CGD-CBD	-2.75	118.78	124.42
13	A	813	CLA	C1-O2A-CGA	2.75	124.68	116.98
13	A	835	CLA	C3B-CAB-CBB	-2.75	120.25	125.95
13	A	805	CLA	O1D-CGD-CBD	-2.75	118.80	124.42
15	A	851	BCR	C8-C7-C6	-2.75	119.21	127.32
15	B	846	BCR	C27-C26-C25	-2.75	119.18	122.84
15	M	1203	BCR	C12-C13-C14	-2.75	114.75	118.97
13	B	824	CLA	O2A-CGA-CBA	2.74	120.57	111.94
15	F	1302	BCR	C34-C9-C10	-2.74	119.03	122.92
13	B	821	CLA	C3B-CAB-CBB	-2.74	120.28	125.95
13	A	809	CLA	C2A-C1A-NA	-2.74	108.21	111.24
13	B	839	CLA	O1D-CGD-CBD	-2.74	118.81	124.42
13	A	845	CLA	O2D-CGD-O1D	-2.74	118.23	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	851	BCR	C29-C30-C25	2.74	114.99	110.44
13	A	839	CLA	O2A-CGA-CBA	2.74	120.55	111.94
13	A	821	CLA	O2A-CGA-CBA	2.73	120.54	111.94
13	B	828	CLA	O1D-CGD-CBD	-2.73	118.82	124.42
15	A	850	BCR	C4-C5-C6	-2.73	119.20	122.84
15	B	841	BCR	C8-C7-C6	-2.73	119.25	127.32
15	B	845	BCR	C7-C8-C9	-2.73	122.13	126.22
13	A	819	CLA	C2C-C1C-NC	-2.73	107.95	110.17
13	A	816	CLA	C3B-CAB-CBB	-2.73	120.30	125.95
13	A	823	CLA	C1D-C2D-C3D	-2.73	104.55	106.78
15	B	847	BCR	C10-C11-C12	-2.73	114.04	123.24
13	A	814	CLA	CAA-CBA-CGA	-2.73	105.24	112.75
13	A	825	CLA	C4-C3-C5	2.73	119.53	115.39
13	B	817	CLA	C3B-CAB-CBB	-2.72	120.31	125.95
13	X	102	CLA	C3B-CAB-CBB	-2.72	120.31	125.95
15	B	843	BCR	C34-C9-C10	-2.72	119.05	122.92
13	B	809	CLA	C4D-C3D-CAD	-2.72	104.71	108.05
15	B	843	BCR	C8-C7-C6	-2.72	119.29	127.32
13	A	827	CLA	CMD-C2D-C3D	2.72	129.25	124.97
13	A	834	CLA	O2A-CGA-CBA	2.72	120.49	111.94
13	B	801	CLA	C3B-CAB-CBB	-2.72	120.33	125.95
15	L	1005	BCR	C8-C7-C6	-2.72	119.29	127.32
13	B	810	CLA	C3B-CAB-CBB	-2.72	120.33	125.95
13	A	830	CLA	C4D-C3D-CAD	-2.72	104.71	108.05
13	B	819	CLA	C3B-CAB-CBB	-2.72	120.33	125.95
15	A	849	BCR	C24-C23-C22	-2.71	122.15	126.22
13	L	1003	CLA	CGD-CBD-CHA	2.71	120.18	110.96
13	B	835	CLA	C4D-C3D-CAD	-2.71	104.72	108.05
13	A	811	CLA	C3B-CAB-CBB	-2.71	120.34	125.95
13	B	819	CLA	C4D-C3D-CAD	-2.71	104.72	108.05
16	A	853	LHG	O8-C23-C24	2.71	120.46	111.94
13	A	809	CLA	C2C-C1C-NC	-2.71	107.98	110.17
13	B	825	CLA	O2A-C1-C2	-2.70	102.69	108.55
13	A	809	CLA	C3B-CAB-CBB	-2.70	120.35	125.95
13	J	1101	CLA	O1D-CGD-CBD	-2.70	118.89	124.42
13	A	819	CLA	C3B-CAB-CBB	-2.70	120.36	125.95
13	A	832	CLA	C3B-CAB-CBB	-2.70	120.36	125.95
13	A	808	CLA	C3B-CAB-CBB	-2.70	120.36	125.95
15	B	847	BCR	C16-C15-C14	-2.70	117.38	123.36
13	A	808	CLA	C4-C3-C5	2.70	119.49	115.39
13	I	101	CLA	C3B-CAB-CBB	-2.70	120.36	125.95
13	B	806	CLA	CAA-CBA-CGA	-2.70	104.57	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	1006	BCR	C15-C14-C13	-2.70	123.41	127.29
13	B	814	CLA	C1-O2A-CGA	2.69	124.53	116.98
13	B	816	CLA	C3B-CAB-CBB	-2.69	120.37	125.95
15	L	1006	BCR	C33-C5-C4	2.69	118.28	113.34
15	L	1006	BCR	C10-C11-C12	-2.69	114.15	123.24
13	A	816	CLA	CBD-CHA-C1A	2.69	132.29	128.77
13	A	801	CLA	C4D-C3D-CAD	-2.69	104.74	108.05
15	A	851	BCR	C11-C10-C9	-2.69	123.42	127.29
13	J	1102	CLA	C4D-C3D-CAD	-2.69	104.75	108.05
13	B	836	CLA	C1-O2A-CGA	2.69	124.51	116.98
13	B	808	CLA	C3B-CAB-CBB	-2.69	120.39	125.95
15	B	850	BCR	C29-C30-C25	2.68	114.90	110.44
13	A	812	CLA	C3B-CAB-CBB	-2.68	120.40	125.95
13	A	818	CLA	CAA-C2A-C3A	-2.68	106.71	113.04
13	A	821	CLA	C4-C3-C5	2.68	119.46	115.39
13	F	1301	CLA	OBD-CAD-C3D	-2.68	122.93	127.91
13	B	822	CLA	CMB-C2B-C1B	-2.68	124.50	128.62
13	A	843	CLA	C1-O2A-CGA	2.67	124.47	116.98
13	M	1201	CLA	C5-C6-C7	-2.67	108.23	113.25
13	B	803	CLA	O2A-CGA-CBA	2.67	120.34	111.94
13	A	808	CLA	O1D-CGD-CBD	-2.67	118.96	124.42
13	A	812	CLA	O2D-CGD-O1D	-2.67	118.37	123.79
13	A	810	CLA	C3B-CAB-CBB	-2.66	120.44	125.95
13	A	844	CLA	C1D-CHD-C4C	2.66	126.73	122.60
13	B	813	CLA	C2C-C1C-NC	-2.66	108.01	110.17
13	J	1101	CLA	O2D-CGD-O1D	-2.66	118.39	123.79
13	L	1002	CLA	C2C-C1C-NC	-2.66	108.02	110.17
13	L	1004	CLA	O1D-CGD-CBD	-2.65	118.98	124.42
13	B	820	CLA	C3D-CAD-CBD	-2.66	103.84	107.60
13	A	824	CLA	C2C-C1C-NC	-2.65	108.02	110.17
15	L	1006	BCR	C37-C22-C21	-2.65	119.15	122.92
13	A	813	CLA	CBD-CHA-C1A	2.65	132.23	128.77
13	A	821	CLA	C3D-CAD-CBD	-2.65	103.85	107.60
13	A	838	CLA	C11-C10-C8	-2.64	107.52	115.14
13	A	819	CLA	O2A-C1-C2	-2.64	102.82	108.55
15	J	1104	BCR	C11-C10-C9	-2.64	123.48	127.29
15	B	845	BCR	C16-C17-C18	-2.64	123.49	127.29
13	B	821	CLA	CAA-C2A-C3A	-2.64	106.80	113.04
13	A	809	CLA	C1D-CHD-C4C	2.64	126.69	122.60
13	A	830	CLA	O1D-CGD-CBD	-2.64	119.01	124.42
13	L	1003	CLA	C2C-C1C-NC	-2.64	108.03	110.17
13	B	816	CLA	O1D-CGD-CBD	-2.64	119.02	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	833	CLA	C3B-CAB-CBB	-2.64	120.49	125.95
13	A	820	CLA	CBD-CHA-C1A	2.63	132.21	128.77
13	B	801	CLA	C4D-C3D-CAD	-2.63	104.81	108.05
13	F	1301	CLA	C2A-C1A-CHA	2.63	128.39	123.83
13	M	1201	CLA	O2D-CGD-O1D	-2.63	118.44	123.79
15	J	1104	BCR	C10-C11-C12	-2.63	114.36	123.24
13	A	842	CLA	O2D-CGD-CBD	2.63	116.69	111.33
15	B	849	BCR	C8-C7-C6	-2.63	119.55	127.32
13	B	812	CLA	CAA-CBA-CGA	-2.63	104.79	113.27
15	A	851	BCR	C15-C16-C17	-2.63	117.54	123.36
15	A	849	BCR	C12-C13-C14	-2.63	114.93	118.97
13	J	1102	CLA	O2D-CGD-O1D	-2.63	118.45	123.79
13	B	801	CLA	O2A-CGA-CBA	2.63	120.21	111.94
13	A	843	CLA	C3B-CAB-CBB	-2.63	120.51	125.95
13	A	840	CLA	C3B-CAB-CBB	-2.62	120.52	125.95
14	B	840	PQN	C14-C13-C15	2.62	119.38	115.39
13	A	804	CLA	C3B-CAB-CBB	-2.62	120.52	125.95
13	A	808	CLA	CBD-CHA-C1A	2.62	132.19	128.77
13	L	1004	CLA	C1D-CHD-C4C	2.62	126.66	122.60
13	B	820	CLA	C3B-CAB-CBB	-2.62	120.52	125.95
13	B	830	CLA	C1-C2-C3	-2.62	121.53	126.19
13	A	835	CLA	C2C-C1C-NC	-2.62	108.05	110.17
13	A	832	CLA	C1D-CHD-C4C	2.62	126.66	122.60
15	B	849	BCR	C34-C9-C10	-2.61	119.21	122.92
13	A	811	CLA	O2A-CGA-CBA	2.61	120.16	111.94
13	B	821	CLA	CGD-CBD-CHA	2.61	119.84	110.96
13	A	835	CLA	CGD-CBD-CHA	2.61	119.84	110.96
16	X	101	LHG	C10-C9-C8	-2.61	108.60	114.46
13	A	802	CLA	O2A-CGA-CBA	2.61	120.14	111.94
13	B	815	CLA	C1-O2A-CGA	2.60	124.27	116.98
13	A	842	CLA	C3B-CAB-CBB	-2.60	120.56	125.95
13	B	815	CLA	C3B-CAB-CBB	-2.60	120.57	125.95
13	B	823	CLA	O1D-CGD-CBD	-2.60	119.10	124.42
15	A	847	BCR	C8-C7-C6	-2.59	119.66	127.32
13	A	826	CLA	O2A-CGA-CBA	2.59	120.10	111.94
13	B	830	CLA	C1D-CHD-C4C	2.59	126.62	122.60
13	F	1301	CLA	CAA-C2A-C3A	-2.59	106.91	113.04
13	A	841	CLA	C1D-CHD-C4C	2.59	126.62	122.60
13	B	826	CLA	C1-O2A-CGA	2.59	124.24	116.98
13	B	831	CLA	O2A-CGA-CBA	2.59	120.08	111.94
13	A	802	CLA	C4D-CHA-CBD	-2.59	103.28	109.37
13	L	1003	CLA	C4D-C3D-CAD	-2.59	104.87	108.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	849	BCR	C11-C10-C9	-2.59	123.57	127.29
15	B	849	BCR	C4-C5-C6	-2.59	119.39	122.84
15	B	841	BCR	C12-C13-C14	-2.58	115.00	118.97
13	B	824	CLA	O2D-CGD-O1D	-2.58	118.54	123.79
13	F	1301	CLA	CAA-C2A-C1A	2.58	118.07	111.62
13	A	838	CLA	C3B-CAB-CBB	-2.58	120.61	125.95
13	A	827	CLA	C3B-CAB-CBB	-2.58	120.61	125.95
13	A	813	CLA	O2D-CGD-O1D	-2.58	118.55	123.79
13	B	823	CLA	C1D-CHD-C4C	2.58	126.60	122.60
15	A	852	BCR	C11-C10-C9	-2.58	123.58	127.29
13	A	805	CLA	O2D-CGD-O1D	-2.58	118.55	123.79
13	A	802	CLA	O2D-CGD-O1D	-2.58	118.55	123.79
15	A	848	BCR	C15-C14-C13	-2.58	123.58	127.29
15	M	1203	BCR	C23-C24-C25	-2.58	119.71	127.32
13	A	830	CLA	C2C-C1C-NC	-2.58	108.08	110.17
13	A	802	CLA	C1D-CHD-C4C	2.57	126.59	122.60
15	I	102	BCR	C29-C30-C25	2.57	114.71	110.44
15	L	1005	BCR	C21-C20-C19	-2.57	114.58	123.24
13	A	839	CLA	C3B-CAB-CBB	-2.57	120.64	125.95
13	A	840	CLA	C4-C3-C5	2.56	119.29	115.39
15	A	848	BCR	C8-C7-C6	-2.56	119.75	127.32
13	B	814	CLA	C4D-C3D-CAD	-2.56	104.90	108.05
13	B	824	CLA	C3B-CAB-CBB	-2.56	120.65	125.95
15	B	843	BCR	C39-C30-C25	-2.56	106.09	110.33
13	B	816	CLA	C2C-C1C-NC	-2.56	108.09	110.17
15	A	848	BCR	C27-C26-C25	-2.56	119.43	122.84
15	A	849	BCR	C15-C16-C17	-2.56	117.70	123.36
13	A	845	CLA	C1D-CHD-C4C	2.56	126.56	122.60
13	A	836	CLA	O1D-CGD-CBD	-2.56	119.19	124.42
13	A	822	CLA	O2A-CGA-CBA	2.55	119.97	111.94
13	B	803	CLA	C1-C2-C3	-2.55	121.64	126.19
13	A	855	CLA	C1D-CHD-C4C	2.55	126.56	122.60
13	B	834	CLA	C1D-CHD-C4C	2.55	126.56	122.60
15	A	848	BCR	C12-C13-C14	-2.55	115.05	118.97
13	B	819	CLA	O2D-CGD-O1D	-2.55	118.61	123.79
15	B	847	BCR	C23-C24-C25	-2.55	119.80	127.32
15	B	843	BCR	C36-C18-C17	-2.55	119.31	122.92
13	A	833	CLA	O2A-CGA-CBA	2.54	119.94	111.94
15	A	852	BCR	C27-C26-C25	-2.54	119.45	122.84
13	L	1004	CLA	C1-C2-C3	-2.54	121.67	126.19
13	A	827	CLA	C1-C2-C3	-2.54	121.67	126.19
13	B	806	CLA	C3B-CAB-CBB	-2.54	120.70	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	1101	CLA	C3B-CAB-CBB	-2.54	120.70	125.95
15	A	851	BCR	C36-C18-C17	-2.53	119.32	122.92
13	J	1102	CLA	C2C-C1C-NC	-2.53	108.12	110.17
15	A	849	BCR	C27-C26-C25	-2.53	119.47	122.84
13	B	811	CLA	O2D-CGD-O1D	-2.53	118.65	123.79
13	A	809	CLA	O2D-CGD-O1D	-2.53	118.65	123.79
15	B	849	BCR	C24-C23-C22	-2.53	122.43	126.22
13	A	812	CLA	C5-C6-C7	-2.53	108.50	113.25
13	A	804	CLA	O2D-CGD-O1D	-2.53	118.65	123.79
13	B	818	CLA	C2C-C1C-NC	-2.53	108.12	110.17
15	J	1104	BCR	C23-C24-C25	-2.52	119.86	127.32
13	B	813	CLA	C4D-C3D-CAD	-2.52	104.95	108.05
13	B	839	CLA	C1D-CHD-C4C	2.52	126.51	122.60
15	J	1105	BCR	C10-C11-C12	-2.52	114.73	123.24
13	A	831	CLA	O2A-CGA-CBA	2.52	119.88	111.94
13	A	855	CLA	CBD-CHA-C1A	2.52	132.07	128.77
15	I	102	BCR	C15-C16-C17	-2.52	117.78	123.36
13	A	841	CLA	C3B-CAB-CBB	-2.52	120.73	125.95
13	M	1202	CLA	C3B-CAB-CBB	-2.52	120.74	125.95
13	A	827	CLA	O1D-CGD-CBD	-2.52	119.27	124.42
13	B	803	CLA	C3B-CAB-CBB	-2.51	120.75	125.95
13	A	813	CLA	C3B-CAB-CBB	-2.51	120.75	125.95
15	J	1105	BCR	C27-C26-C25	-2.51	119.49	122.84
15	A	852	BCR	C24-C23-C22	-2.51	122.46	126.22
15	A	852	BCR	C23-C24-C25	-2.51	119.91	127.32
13	A	835	CLA	C5-C6-C7	-2.51	108.54	113.25
13	A	810	CLA	C4D-C3D-CAD	-2.51	104.97	108.05
13	B	838	CLA	O1D-CGD-CBD	-2.51	119.29	124.42
13	B	827	CLA	C2B-C1B-NB	2.50	111.30	109.41
15	B	845	BCR	C23-C24-C25	-2.50	119.92	127.32
15	J	1104	BCR	C24-C23-C22	-2.50	122.47	126.22
13	B	816	CLA	CAA-C2A-C3A	-2.50	107.12	113.04
15	A	851	BCR	C10-C11-C12	-2.50	114.80	123.24
15	A	851	BCR	C23-C24-C25	-2.50	119.94	127.32
13	A	829	CLA	C1D-CHD-C4C	2.50	126.48	122.60
15	A	848	BCR	C23-C24-C25	-2.50	119.94	127.32
15	M	1203	BCR	C15-C16-C17	-2.50	117.83	123.36
15	A	848	BCR	C11-C10-C9	-2.50	123.70	127.29
13	B	828	CLA	O2D-CGD-O1D	-2.50	118.72	123.79
13	B	806	CLA	O1D-CGD-CBD	-2.49	119.31	124.42
15	B	841	BCR	C4-C5-C6	-2.49	119.52	122.84
13	A	811	CLA	C2C-C1C-NC	-2.49	108.15	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	814	CLA	C2C-C1C-NC	-2.49	108.15	110.17
13	M	1201	CLA	C1-C2-C3	-2.49	121.77	126.19
13	B	835	CLA	CBD-CHA-C1A	2.49	132.02	128.77
13	B	823	CLA	CBD-CHA-C1A	2.48	132.02	128.77
13	B	802	CLA	C4-C3-C2	-2.49	118.60	123.52
15	A	848	BCR	C4-C5-C6	-2.48	119.53	122.84
13	B	836	CLA	C2C-C1C-NC	-2.48	108.16	110.17
15	B	845	BCR	C4-C5-C6	-2.48	119.53	122.84
13	B	825	CLA	C3B-CAB-CBB	-2.48	120.81	125.95
13	B	835	CLA	CGD-CBD-CHA	2.48	119.39	110.96
13	A	803	CLA	C1D-CHD-C4C	2.48	126.45	122.60
13	A	803	CLA	O2A-CGA-CBA	2.48	119.74	111.94
13	A	816	CLA	C1D-CHD-C4C	2.48	126.44	122.60
13	A	838	CLA	C1-O2A-CGA	2.48	123.92	116.98
13	B	831	CLA	C3B-CAB-CBB	-2.48	120.82	125.95
15	J	1104	BCR	C4-C5-C6	-2.48	119.54	122.84
15	B	846	BCR	C16-C15-C14	-2.48	117.88	123.36
15	F	1302	BCR	C27-C26-C25	-2.48	119.54	122.84
13	A	820	CLA	C1D-CHD-C4C	2.48	126.44	122.60
15	B	844	BCR	C16-C17-C18	-2.48	123.72	127.29
13	J	1101	CLA	C1D-CHD-C4C	2.47	126.44	122.60
13	B	823	CLA	O2A-CGA-O1A	-2.47	117.84	122.96
15	B	847	BCR	C31-C1-C6	-2.47	106.23	110.33
13	A	831	CLA	C4D-C3D-CAD	-2.47	105.01	108.05
13	A	829	CLA	O2D-CGD-O1D	-2.47	118.77	123.79
15	A	848	BCR	C10-C11-C12	-2.47	114.91	123.24
13	A	821	CLA	C1D-CHD-C4C	2.47	126.42	122.60
13	A	806	CLA	C1D-CHD-C4C	2.46	126.42	122.60
13	A	833	CLA	C3B-CAB-CBB	-2.46	120.85	125.95
13	M	1202	CLA	C1D-CHD-C4C	2.46	126.42	122.60
13	B	835	CLA	C2A-C1A-CHA	2.46	128.09	123.83
13	B	803	CLA	C2C-C1C-NC	-2.46	108.18	110.17
15	B	850	BCR	C35-C13-C12	2.46	122.07	118.09
13	A	845	CLA	C2C-C1C-NC	-2.46	108.18	110.17
13	B	809	CLA	CAA-CBA-CGA	-2.46	105.97	112.75
13	A	818	CLA	CAA-CBA-CGA	-2.46	105.34	113.27
13	A	813	CLA	C1D-CHD-C4C	2.46	126.41	122.60
13	B	814	CLA	C3B-CAB-CBB	-2.45	120.87	125.95
13	B	807	CLA	C3B-CAB-CBB	-2.45	120.87	125.95
13	A	804	CLA	OBD-CAD-C3D	-2.45	123.34	127.91
13	B	834	CLA	C4D-C3D-CAD	-2.45	105.03	108.05
13	B	813	CLA	C1D-CHD-C4C	2.45	126.40	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	848	LMG	C7-O1-C1	2.45	118.69	113.81
15	A	849	BCR	C16-C15-C14	-2.45	117.94	123.36
13	B	832	CLA	C2C-C1C-NC	-2.45	108.19	110.17
13	A	820	CLA	C2A-C3A-C4A	2.45	105.16	101.40
13	B	822	CLA	C1D-CHD-C4C	2.45	126.39	122.60
13	A	815	CLA	C1D-CHD-C4C	2.44	126.39	122.60
13	A	809	CLA	CMD-C2D-C3D	2.45	128.82	124.97
13	M	1201	CLA	O2A-CGA-CBA	2.44	119.62	111.94
15	L	1006	BCR	C4-C5-C6	-2.44	119.59	122.84
13	A	821	CLA	C3B-CAB-CBB	-2.44	120.90	125.95
13	A	845	CLA	C1-O2A-CGA	2.44	123.81	116.98
13	A	832	CLA	C2C-C1C-NC	-2.44	108.19	110.17
13	B	815	CLA	CBD-CHA-C1A	2.44	131.96	128.77
15	B	843	BCR	C12-C13-C14	-2.44	115.22	118.97
15	A	850	BCR	C27-C26-C25	-2.44	119.59	122.84
13	A	826	CLA	C1D-CHD-C4C	2.44	126.38	122.60
13	B	805	CLA	C3D-CAD-CBD	-2.43	104.16	107.60
13	A	833	CLA	C4D-C3D-CAD	-2.43	105.06	108.05
15	B	844	BCR	C27-C26-C25	-2.43	119.60	122.84
13	A	827	CLA	C4D-C3D-CAD	-2.43	105.06	108.05
15	J	1105	BCR	C4-C5-C6	-2.43	119.60	122.84
13	B	834	CLA	O2D-CGD-O1D	-2.43	118.85	123.79
15	A	852	BCR	C1-C6-C7	2.43	122.41	115.69
13	A	803	CLA	C2C-C1C-NC	-2.43	108.20	110.17
13	B	805	CLA	C3B-CAB-CBB	-2.43	120.93	125.95
13	A	814	CLA	O1D-CGD-CBD	-2.42	119.45	124.42
15	M	1203	BCR	C7-C8-C9	-2.42	122.59	126.22
15	A	847	BCR	C4-C5-C6	-2.42	119.61	122.84
15	J	1105	BCR	C23-C24-C25	-2.42	120.17	127.32
15	L	1005	BCR	C10-C11-C12	-2.42	115.07	123.24
15	A	848	BCR	C36-C18-C17	-2.42	119.48	122.92
13	B	807	CLA	O2D-CGD-O1D	-2.42	118.87	123.79
13	A	836	CLA	C1D-CHD-C4C	2.42	126.35	122.60
13	A	844	CLA	C2C-C1C-NC	-2.42	108.21	110.17
13	B	804	CLA	CAA-C2A-C1A	2.42	117.66	111.62
13	A	812	CLA	C1D-CHD-C4C	2.42	126.35	122.60
13	I	101	CLA	CGD-CBD-CHA	2.41	119.17	110.96
13	A	828	CLA	C2C-C1C-NC	-2.41	108.21	110.17
13	A	815	CLA	CBD-CHA-C1A	2.41	131.92	128.77
13	B	802	CLA	CAA-C2A-C1A	2.41	117.64	111.62
13	B	818	CLA	C1D-CHD-C4C	2.41	126.34	122.60
13	B	817	CLA	O2A-CGA-CBA	2.41	119.52	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	811	CLA	C3B-CAB-CBB	-2.41	120.96	125.95
13	A	816	CLA	C4D-C3D-CAD	-2.41	105.09	108.05
15	A	847	BCR	C15-C14-C13	-2.41	123.82	127.29
13	B	821	CLA	C2C-C1C-NC	-2.41	108.22	110.17
13	A	817	CLA	C5-C6-C7	-2.41	108.73	113.25
13	A	838	CLA	O2D-CGD-O1D	-2.41	118.90	123.79
13	A	841	CLA	C1-C2-C3	-2.40	121.91	126.19
15	J	1104	BCR	C15-C16-C17	-2.40	118.04	123.36
13	B	827	CLA	C3B-CAB-CBB	-2.40	120.98	125.95
13	A	836	CLA	O2D-CGD-O1D	-2.40	118.91	123.79
14	A	846	PQN	C14-C13-C15	2.40	119.04	115.39
13	A	803	CLA	C11-C12-C13	-2.40	108.23	115.14
13	A	819	CLA	C1-O2A-CGA	2.40	123.70	116.98
15	L	1005	BCR	C27-C26-C25	-2.40	119.65	122.84
13	A	844	CLA	C1D-C2D-C3D	-2.40	104.82	106.78
13	B	805	CLA	CBD-CHA-C1A	2.40	131.90	128.77
13	B	822	CLA	O2A-CGA-CBA	2.40	119.47	111.94
13	B	815	CLA	C10-C11-C12	-2.40	109.94	114.68
15	A	850	BCR	C37-C22-C21	-2.39	119.52	122.92
13	I	101	CLA	C1-O2A-CGA	2.39	123.69	116.98
13	M	1201	CLA	C1D-CHD-C4C	2.39	126.31	122.60
13	B	835	CLA	O1D-CGD-CBD	-2.39	119.52	124.42
13	B	825	CLA	C2A-C3A-C4A	2.39	105.08	101.40
13	J	1101	CLA	CBA-CAA-C2A	2.39	121.11	114.01
13	A	819	CLA	O2A-CGA-CBA	2.39	119.46	111.94
13	B	837	CLA	O2A-CGA-CBA	2.39	119.45	111.94
13	J	1102	CLA	C1D-CHD-C4C	2.39	126.31	122.60
13	A	841	CLA	C4-C3-C5	2.39	120.23	114.77
13	A	843	CLA	O2A-C1-C2	-2.39	103.38	108.55
13	A	830	CLA	C1-O2A-CGA	2.39	123.67	116.98
13	B	811	CLA	C4D-C3D-CAD	-2.38	105.12	108.05
13	A	838	CLA	CAA-C2A-C1A	2.38	117.57	111.62
13	B	807	CLA	C11-C10-C8	-2.38	108.28	115.14
13	B	810	CLA	CAA-C2A-C1A	-2.38	105.68	111.62
15	A	849	BCR	C37-C22-C21	-2.38	119.54	122.92
13	B	805	CLA	O2A-CGA-CBA	2.38	119.42	111.94
13	A	836	CLA	C3D-CAD-CBD	-2.38	104.23	107.60
13	A	813	CLA	C2C-C1C-NC	-2.38	108.24	110.17
13	B	808	CLA	C1D-CHD-C4C	2.38	126.28	122.60
13	A	843	CLA	CMD-C2D-C3D	2.38	128.71	124.97
13	B	820	CLA	CAA-C2A-C1A	2.37	117.55	111.62
13	B	810	CLA	C1D-CHD-C4C	2.37	126.28	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	821	CLA	C2C-C1C-NC	-2.37	108.25	110.17
13	B	814	CLA	C4-C3-C5	2.37	118.99	115.39
13	B	811	CLA	C1D-CHD-C4C	2.37	126.27	122.60
13	A	838	CLA	C2C-C1C-NC	-2.37	108.25	110.17
13	A	829	CLA	C4D-C3D-CAD	-2.37	105.14	108.05
13	B	838	CLA	C2C-C1C-NC	-2.37	108.25	110.17
13	A	855	CLA	C4D-C3D-CAD	-2.37	105.14	108.05
13	A	823	CLA	C3B-CAB-CBB	-2.36	121.06	125.95
13	A	826	CLA	C2C-C1C-NC	-2.36	108.25	110.17
13	L	1004	CLA	CAA-C2A-C1A	2.36	117.52	111.62
13	J	1103	CLA	C1D-CHD-C4C	2.36	126.26	122.60
13	A	826	CLA	C1-C2-C3	-2.36	121.98	126.19
13	A	801	CLA	CAA-C2A-C1A	2.36	117.52	111.62
15	B	847	BCR	C37-C22-C21	-2.36	119.57	122.92
13	L	1002	CLA	C1D-CHD-C4C	2.36	126.26	122.60
13	A	822	CLA	CAA-C2A-C1A	2.36	117.51	111.62
13	X	102	CLA	C4D-C3D-CAD	-2.36	105.15	108.05
13	A	855	CLA	O2D-CGD-O1D	-2.36	119.00	123.79
15	A	852	BCR	C10-C11-C12	-2.35	115.30	123.24
13	A	835	CLA	C1D-CHD-C4C	2.35	126.25	122.60
13	A	837	CLA	C4D-C3D-CAD	-2.35	105.16	108.05
13	A	835	CLA	O2A-CGA-CBA	2.35	119.34	111.94
13	B	833	CLA	C1D-CHD-C4C	2.35	126.24	122.60
13	A	808	CLA	C2C-C1C-NC	-2.35	108.27	110.17
13	B	801	CLA	O2D-CGD-O1D	-2.35	119.02	123.79
13	A	833	CLA	C1D-CHD-C4C	2.35	126.24	122.60
14	B	840	PQN	C2M-C2-C1	2.35	120.44	116.33
15	B	845	BCR	C40-C30-C25	-2.35	106.44	110.33
13	B	815	CLA	C1D-CHD-C4C	2.35	126.24	122.60
13	B	838	CLA	C4D-C3D-CAD	-2.34	105.17	108.05
13	A	808	CLA	OBD-CAD-CBD	-2.34	122.40	125.94
13	B	801	CLA	C2A-C3A-C4A	2.34	105.00	101.40
13	A	802	CLA	C2C-C1C-NC	-2.34	108.27	110.17
13	B	816	CLA	O2A-CGA-CBA	2.34	119.30	111.94
13	A	820	CLA	O2D-CGD-O1D	-2.34	119.04	123.79
13	B	809	CLA	C3B-CAB-CBB	-2.34	121.11	125.95
13	A	840	CLA	C1-O2A-CGA	2.34	123.52	116.98
15	B	845	BCR	C29-C28-C27	2.33	117.43	111.48
13	L	1002	CLA	O2D-CGD-O1D	-2.33	119.05	123.79
15	A	847	BCR	C12-C13-C14	-2.33	115.39	118.97
13	A	813	CLA	C4D-C3D-CAD	-2.33	105.18	108.05
13	A	828	CLA	C4D-C3D-CAD	-2.33	105.19	108.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	842	CLA	C1-C2-C3	-2.33	122.04	126.19
13	B	836	CLA	O2D-CGD-O1D	-2.33	119.06	123.79
13	L	1002	CLA	C3B-CAB-CBB	-2.33	121.13	125.95
13	A	813	CLA	C11-C12-C13	-2.33	108.93	114.92
15	B	846	BCR	C4-C5-C6	-2.33	119.74	122.84
15	B	846	BCR	C8-C9-C10	-2.32	115.40	118.97
13	X	102	CLA	CAA-C2A-C1A	2.32	117.43	111.62
13	B	832	CLA	CAA-CBA-CGA	-2.32	106.35	112.75
13	A	834	CLA	C3D-CAD-CBD	-2.32	104.31	107.60
13	A	839	CLA	CBD-CHA-C1A	2.32	131.81	128.77
13	A	843	CLA	C1D-CHD-C4C	2.32	126.20	122.60
13	B	836	CLA	C1D-CHD-C4C	2.32	126.20	122.60
13	B	831	CLA	CBD-CHA-C1A	2.32	131.80	128.77
13	B	802	CLA	C2C-C1C-NC	-2.32	108.29	110.17
13	M	1202	CLA	O2D-CGD-O1D	-2.32	119.08	123.79
13	A	818	CLA	C1D-CHD-C4C	2.32	126.19	122.60
13	B	833	CLA	CBD-CHA-C1A	2.31	131.80	128.77
13	A	805	CLA	C4-C3-C5	2.31	118.91	115.39
13	A	824	CLA	C10-C11-C12	-2.31	110.10	114.68
13	A	839	CLA	C1D-CHD-C4C	2.31	126.19	122.60
13	B	814	CLA	C4B-CHC-C1C	-2.31	124.43	127.47
13	B	835	CLA	O2D-CGD-O1D	-2.31	119.10	123.79
13	B	819	CLA	C1D-CHD-C4C	2.31	126.18	122.60
13	A	801	CLA	O2A-CGA-CBA	2.31	119.19	111.94
13	J	1102	CLA	C3B-CAB-CBB	-2.31	121.18	125.95
13	B	821	CLA	O2D-CGD-CBD	2.31	116.03	111.33
13	B	820	CLA	C1D-CHD-C4C	2.31	126.17	122.60
13	A	840	CLA	C1-C2-C3	-2.30	122.09	126.19
13	B	830	CLA	CAA-CBA-CGA	-2.30	105.84	113.27
15	B	849	BCR	C29-C30-C25	2.30	114.27	110.44
13	B	812	CLA	C1-O2A-CGA	2.30	123.42	116.98
13	B	810	CLA	C2C-C1C-NC	-2.30	108.30	110.17
13	B	820	CLA	C2C-C1C-NC	-2.30	108.31	110.17
13	A	816	CLA	C2C-C1C-NC	-2.30	108.31	110.17
13	A	825	CLA	O2A-CGA-CBA	2.30	119.18	111.94
15	J	1104	BCR	C37-C22-C21	-2.30	119.66	122.92
13	B	828	CLA	C1D-CHD-C4C	2.30	126.16	122.60
13	B	803	CLA	OBD-CAD-CBD	2.30	129.40	125.94
15	L	1006	BCR	C12-C13-C14	-2.30	115.44	118.97
13	B	824	CLA	C1D-CHD-C4C	2.30	126.16	122.60
15	L	1005	BCR	C4-C5-C6	-2.30	119.78	122.84
13	A	801	CLA	C4B-CHC-C1C	-2.29	124.45	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	843	CLA	C2C-C1C-NC	-2.29	108.31	110.17
13	A	828	CLA	C1-O2A-CGA	2.29	123.39	116.98
15	B	842	BCR	C34-C9-C10	-2.29	119.67	122.92
15	B	850	BCR	C34-C9-C10	-2.29	119.67	122.92
13	A	843	CLA	C4D-C3D-CAD	-2.29	105.24	108.05
13	B	838	CLA	O2D-CGD-O1D	-2.29	119.14	123.79
13	B	828	CLA	C4D-C3D-CAD	-2.29	105.24	108.05
15	B	842	BCR	C37-C22-C21	-2.28	119.68	122.92
15	B	843	BCR	C21-C20-C19	-2.28	115.53	123.24
13	B	814	CLA	C7-C6-C5	-2.28	106.28	113.01
15	B	846	BCR	C23-C24-C25	-2.28	120.58	127.32
15	B	850	BCR	C36-C18-C17	-2.28	119.68	122.92
13	A	836	CLA	CMD-C2D-C3D	2.28	128.57	124.97
13	L	1004	CLA	C2C-C1C-NC	-2.28	108.32	110.17
13	B	806	CLA	C4-C3-C2	-2.28	119.00	123.52
13	A	837	CLA	C1D-CHD-C4C	2.28	126.14	122.60
13	A	825	CLA	C2A-C3A-C4A	2.28	104.91	101.40
13	A	825	CLA	O2A-C1-C2	-2.28	103.61	108.55
13	B	816	CLA	C1D-CHD-C4C	2.28	126.13	122.60
13	A	819	CLA	O2D-CGD-O1D	-2.28	119.16	123.79
13	A	826	CLA	O2D-CGD-O1D	-2.28	119.16	123.79
13	A	803	CLA	C3B-CAB-CBB	-2.28	121.24	125.95
13	A	821	CLA	C4-C3-C2	-2.28	119.01	123.52
13	B	837	CLA	C1D-CHD-C4C	2.27	126.13	122.60
13	B	815	CLA	C2C-C1C-NC	-2.27	108.33	110.17
15	B	850	BCR	C10-C11-C12	-2.27	115.57	123.24
13	B	824	CLA	C4D-C3D-CAD	-2.27	105.26	108.05
13	B	838	CLA	C1D-CHD-C4C	2.27	126.12	122.60
15	L	1005	BCR	C30-C25-C24	2.27	121.98	115.69
15	A	850	BCR	C16-C15-C14	-2.27	118.33	123.36
13	L	1003	CLA	C1D-CHD-C4C	2.27	126.12	122.60
13	A	807	CLA	C4D-C3D-CAD	-2.27	105.26	108.05
15	B	847	BCR	C27-C26-C25	-2.27	119.82	122.84
13	B	817	CLA	C1D-CHD-C4C	2.27	126.12	122.60
13	A	839	CLA	O1D-CGD-CBD	-2.27	119.78	124.42
13	A	819	CLA	C1D-CHD-C4C	2.27	126.11	122.60
13	A	825	CLA	C1D-CHD-C4C	2.27	126.11	122.60
13	B	832	CLA	C1D-CHD-C4C	2.27	126.11	122.60
13	A	806	CLA	C2C-C1C-NC	-2.26	108.33	110.17
15	A	847	BCR	C34-C9-C10	-2.26	119.70	122.92
13	A	845	CLA	C4D-C3D-CAD	-2.26	105.27	108.05
13	A	813	CLA	C11-C10-C8	-2.27	108.61	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	812	CLA	C2C-C1C-NC	-2.27	108.33	110.17
15	L	1005	BCR	C15-C14-C13	-2.26	124.03	127.29
13	B	816	CLA	C7-C6-C5	-2.26	106.34	113.01
13	X	102	CLA	C1D-CHD-C4C	2.26	126.10	122.60
13	A	837	CLA	C3B-CAB-CBB	-2.26	121.28	125.95
13	A	817	CLA	C1-O2A-CGA	2.26	123.30	116.98
13	B	834	CLA	CAA-C2A-C1A	2.25	117.25	111.62
15	B	846	BCR	C37-C22-C21	-2.25	119.72	122.92
15	B	842	BCR	C16-C17-C18	-2.25	124.05	127.29
13	B	816	CLA	C4D-C3D-CAD	-2.25	105.29	108.05
13	A	811	CLA	C4D-C3D-CAD	-2.25	105.29	108.05
13	X	102	CLA	C2C-C1C-NC	-2.25	108.35	110.17
13	A	822	CLA	C2C-C1C-NC	-2.25	108.35	110.17
13	A	840	CLA	CAA-CBA-CGA	-2.25	106.02	113.27
15	L	1006	BCR	C16-C15-C14	-2.25	118.39	123.36
13	B	835	CLA	C1-C2-C3	-2.24	122.20	126.19
15	A	848	BCR	C16-C15-C14	-2.24	118.40	123.36
13	B	810	CLA	CED-O2D-CGD	2.24	121.35	116.02
15	B	846	BCR	C39-C30-C25	-2.24	106.62	110.33
13	B	818	CLA	C4D-C3D-CAD	-2.24	105.30	108.05
13	J	1101	CLA	C2A-C3A-C4A	2.24	104.84	101.40
13	A	823	CLA	C4-C3-C5	2.24	119.88	114.77
13	A	817	CLA	CED-O2D-CGD	2.24	121.34	116.02
13	A	838	CLA	C1D-CHD-C4C	2.23	126.06	122.60
13	A	806	CLA	C11-C10-C8	-2.23	108.71	115.14
15	I	102	BCR	C27-C26-C25	-2.23	119.86	122.84
15	M	1203	BCR	C2-C3-C4	2.23	117.17	111.48
13	A	808	CLA	CMD-C2D-C3D	2.23	128.49	124.97
15	B	843	BCR	C2-C3-C4	2.23	117.17	111.48
13	B	828	CLA	C4B-CHC-C1C	-2.23	124.53	127.47
13	B	817	CLA	C1-C2-C3	-2.23	122.22	126.19
15	J	1104	BCR	C39-C30-C25	-2.23	106.64	110.33
15	B	846	BCR	C36-C18-C17	-2.23	119.75	122.92
13	A	843	CLA	C6-C7-C8	-2.23	108.72	115.14
13	A	842	CLA	CED-O2D-CGD	2.23	121.32	116.02
13	J	1101	CLA	C2C-C1C-NC	-2.23	108.36	110.17
13	B	823	CLA	CBA-CAA-C2A	-2.23	107.40	114.01
13	B	838	CLA	CBA-CAA-C2A	2.23	120.63	114.01
13	A	826	CLA	C11-C10-C8	-2.23	108.72	115.14
15	A	851	BCR	C27-C26-C25	-2.23	119.87	122.84
13	A	843	CLA	CAA-CBA-CGA	-2.23	106.09	113.27
15	B	847	BCR	C36-C18-C17	-2.23	119.76	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	849	BCR	C36-C18-C17	-2.23	119.76	122.92
13	A	824	CLA	C11-C10-C8	-2.22	108.74	115.14
13	A	809	CLA	O1D-CGD-CBD	-2.22	119.87	124.42
13	B	825	CLA	C1D-CHD-C4C	2.22	126.05	122.60
15	J	1104	BCR	C29-C28-C27	2.22	117.14	111.48
13	B	806	CLA	O2A-C1-C2	-2.22	103.74	108.55
15	L	1006	BCR	C27-C26-C25	-2.22	119.88	122.84
13	B	839	CLA	C4D-C3D-CAD	-2.22	105.33	108.05
13	A	821	CLA	C16-C15-C13	-2.22	108.75	115.14
13	B	837	CLA	O2D-CGD-O1D	-2.22	119.29	123.79
15	B	841	BCR	C23-C24-C25	-2.21	120.78	127.32
13	A	811	CLA	C1-C2-C3	-2.21	122.25	126.19
13	A	802	CLA	CGD-CBD-CHA	2.21	118.48	110.96
13	B	822	CLA	CAA-C2A-C1A	2.21	117.15	111.62
13	B	822	CLA	C4D-C3D-CAD	-2.21	105.33	108.05
13	A	823	CLA	C4B-CHC-C1C	-2.21	124.56	127.47
15	B	843	BCR	C11-C10-C9	-2.21	124.11	127.29
13	B	833	CLA	C2C-C1C-NC	-2.21	108.38	110.17
13	B	814	CLA	CAA-CBA-CGA	-2.21	106.14	113.27
13	B	839	CLA	O2A-CGA-CBA	2.21	118.89	111.94
15	A	847	BCR	C36-C18-C17	-2.21	119.78	122.92
13	A	818	CLA	CBD-CHA-C1A	2.21	131.66	128.77
13	A	842	CLA	CAA-C2A-C1A	2.21	117.13	111.62
13	B	820	CLA	C1-O2A-CGA	2.21	123.16	116.98
13	B	808	CLA	CAA-C2A-C1A	2.20	117.12	111.62
13	M	1202	CLA	C4D-C3D-CAD	-2.20	105.34	108.05
15	J	1105	BCR	C37-C22-C21	-2.20	119.79	122.92
15	J	1104	BCR	C12-C13-C14	-2.20	115.59	118.97
13	A	820	CLA	C2C-C1C-NC	-2.20	108.39	110.17
13	B	839	CLA	CAA-CBA-CGA	-2.20	106.18	113.27
13	A	839	CLA	C2C-C1C-NC	-2.20	108.39	110.17
15	B	850	BCR	C32-C1-C6	-2.20	106.69	110.33
13	A	835	CLA	O2D-CGD-O1D	-2.20	119.32	123.79
13	F	1301	CLA	C1D-CHD-C4C	2.20	126.01	122.60
13	A	829	CLA	C2C-C1C-NC	-2.20	108.39	110.17
13	A	845	CLA	C7-C6-C5	-2.19	109.53	114.46
13	A	824	CLA	O2A-CGA-CBA	2.19	118.84	111.94
13	B	811	CLA	O2A-C1-C2	2.19	113.30	108.55
13	B	803	CLA	O2D-CGD-O1D	-2.19	119.34	123.79
15	B	843	BCR	C35-C13-C12	2.19	121.64	118.09
15	B	843	BCR	C16-C15-C14	-2.19	118.51	123.36
13	A	837	CLA	C4-C3-C5	2.19	119.78	114.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	830	CLA	C2A-C3A-C4A	2.19	104.77	101.40
13	B	819	CLA	CAA-C2A-C1A	2.19	117.10	111.62
15	B	841	BCR	C16-C15-C14	-2.19	118.52	123.36
15	A	852	BCR	C8-C7-C6	-2.19	120.86	127.32
13	B	809	CLA	C1D-CHD-C4C	2.19	125.99	122.60
15	B	841	BCR	C37-C22-C21	-2.18	119.82	122.92
13	A	807	CLA	C2C-C1C-NC	-2.18	108.40	110.17
13	A	821	CLA	C2A-C3A-C4A	2.18	104.76	101.40
13	F	1301	CLA	O1D-CGD-CBD	-2.18	119.95	124.42
13	B	837	CLA	C2C-C1C-NC	-2.18	108.40	110.17
13	J	1101	CLA	C11-C10-C8	-2.18	108.86	115.14
13	B	832	CLA	C3B-CAB-CBB	-2.18	121.44	125.95
13	A	801	CLA	C11-C10-C8	-2.18	108.87	115.14
15	B	842	BCR	C31-C1-C6	-2.18	106.72	110.33
13	A	824	CLA	C1D-CHD-C4C	2.18	125.98	122.60
13	B	830	CLA	C2C-C1C-NC	-2.18	108.41	110.17
13	A	804	CLA	C1D-CHD-C4C	2.18	125.98	122.60
13	A	804	CLA	C10-C11-C12	-2.18	110.37	114.68
13	A	809	CLA	CGD-CBD-CAD	-2.18	103.56	110.96
13	A	830	CLA	O2D-CGD-O1D	-2.18	119.37	123.79
15	A	847	BCR	C37-C22-C21	-2.18	119.83	122.92
15	I	102	BCR	C16-C15-C14	-2.18	118.54	123.36
13	A	843	CLA	C11-C10-C8	-2.17	108.88	115.14
15	L	1005	BCR	C36-C18-C19	2.17	121.61	118.09
13	A	831	CLA	O1D-CGD-CBD	-2.17	119.97	124.42
13	A	804	CLA	C2C-C1C-NC	-2.17	108.41	110.17
13	I	101	CLA	C11-C10-C8	-2.17	108.88	115.14
13	B	839	CLA	O2D-CGD-O1D	-2.17	119.38	123.79
13	B	826	CLA	C2C-C1C-NC	-2.17	108.41	110.17
13	B	827	CLA	C1-O2A-CGA	2.17	123.06	116.98
13	B	804	CLA	O2D-CGD-O1D	-2.17	119.38	123.79
15	B	850	BCR	C15-C16-C17	-2.17	118.56	123.36
13	B	821	CLA	C1D-CHD-C4C	2.17	125.96	122.60
13	B	824	CLA	C2C-C1C-NC	-2.17	108.41	110.17
13	B	832	CLA	C4D-C3D-CAD	-2.17	105.39	108.05
13	B	803	CLA	C1D-CHD-C4C	2.17	125.96	122.60
13	A	838	CLA	CAA-CBA-CGA	-2.17	106.28	113.27
13	A	808	CLA	C1D-CHD-C4C	2.17	125.96	122.60
13	B	806	CLA	C1D-CHD-C4C	2.17	125.96	122.60
13	A	839	CLA	CAA-CBA-CGA	-2.17	106.28	113.27
13	B	825	CLA	C2C-C1C-NC	-2.16	108.42	110.17
16	A	854	LHG	O10-C23-C24	-2.16	120.04	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	801	CLA	C2C-C1C-NC	-2.16	108.42	110.17
13	B	801	CLA	CMD-C2D-C3D	2.16	128.37	124.97
13	A	817	CLA	C4D-C3D-CAD	-2.16	105.39	108.05
15	B	849	BCR	C32-C1-C6	-2.16	106.75	110.33
13	A	820	CLA	C4D-C3D-CAD	-2.16	105.40	108.05
13	B	804	CLA	C1D-CHD-C4C	2.16	125.95	122.60
13	A	822	CLA	C4D-C3D-CAD	-2.16	105.40	108.05
13	B	821	CLA	C2A-C3A-C4A	2.16	104.72	101.40
13	A	818	CLA	C2C-C1C-NC	-2.16	108.42	110.17
13	A	816	CLA	CED-O2D-CGD	2.16	121.15	116.02
13	A	832	CLA	CAA-C2A-C3A	-2.16	107.94	113.04
13	A	824	CLA	CGD-CBD-CAD	2.15	118.28	110.96
15	B	844	BCR	C21-C20-C19	-2.15	115.97	123.24
13	B	815	CLA	C11-C10-C8	-2.15	108.94	115.14
13	A	819	CLA	C16-C15-C13	-2.15	108.94	115.14
13	A	809	CLA	C11-C10-C8	-2.15	108.94	115.14
15	A	850	BCR	C36-C18-C17	-2.15	119.87	122.92
15	B	841	BCR	C36-C18-C17	-2.15	119.87	122.92
13	B	829	CLA	C1D-CHD-C4C	2.15	125.94	122.60
13	A	807	CLA	C3A-C2A-C1A	2.15	104.12	101.08
13	A	827	CLA	C2A-C3A-C4A	2.15	104.71	101.40
13	A	804	CLA	O2A-CGA-CBA	2.15	118.70	111.94
15	B	844	BCR	C36-C18-C17	-2.15	119.87	122.92
13	J	1101	CLA	CAA-CBA-CGA	2.15	120.19	113.27
13	L	1003	CLA	O2D-CGD-O1D	-2.15	119.43	123.79
13	B	802	CLA	CMD-C2D-C3D	2.15	128.35	124.97
13	M	1201	CLA	CAA-CBA-CGA	-2.15	106.35	113.27
13	B	829	CLA	C2C-C1C-NC	-2.15	108.43	110.17
13	B	812	CLA	C1D-CHD-C4C	2.15	125.93	122.60
13	B	811	CLA	C2A-C3A-C4A	2.15	104.70	101.40
13	B	823	CLA	C2C-C1C-NC	-2.14	108.43	110.17
13	B	811	CLA	C2C-C1C-NC	-2.14	108.43	110.17
15	A	849	BCR	C35-C13-C12	2.14	121.56	118.09
13	J	1103	CLA	C2C-C1C-NC	-2.14	108.43	110.17
13	B	804	CLA	CMB-C2B-C1B	-2.14	125.32	128.62
13	A	837	CLA	C2C-C1C-NC	-2.14	108.43	110.17
13	A	804	CLA	C1-O2A-CGA	2.14	122.98	116.98
13	A	806	CLA	O2A-CGA-CBA	2.14	118.67	111.94
13	A	801	CLA	C2A-C3A-C4A	2.14	104.69	101.40
13	B	827	CLA	C2A-C3A-C4A	2.14	104.69	101.40
15	B	842	BCR	C36-C18-C17	-2.14	119.88	122.92
15	J	1105	BCR	C15-C16-C17	-2.14	118.62	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	849	BCR	C27-C26-C25	-2.14	119.99	122.84
13	B	814	CLA	C1D-CHD-C4C	2.14	125.91	122.60
13	B	834	CLA	C2C-C1C-NC	-2.14	108.44	110.17
15	B	850	BCR	C27-C26-C25	-2.13	120.00	122.84
13	B	820	CLA	CAA-CBA-CGA	-2.13	106.39	113.27
13	A	833	CLA	CED-O2D-CGD	2.13	121.10	116.02
13	F	1301	CLA	C2A-C1A-NA	-2.14	108.88	111.24
13	B	827	CLA	C3B-C2B-C1B	-2.13	105.75	107.00
15	J	1105	BCR	C36-C18-C17	-2.13	119.89	122.92
13	B	835	CLA	C2A-C3A-C4A	2.13	104.68	101.40
13	A	826	CLA	C2A-C3A-C4A	2.13	104.68	101.40
15	A	850	BCR	C35-C13-C12	2.13	121.53	118.09
13	A	837	CLA	C1-C2-C3	-2.13	122.40	126.19
13	A	841	CLA	C2C-C1C-NC	-2.13	108.44	110.17
13	B	803	CLA	C2A-C3A-C4A	2.13	104.67	101.40
13	M	1201	CLA	CAA-C2A-C1A	-2.13	106.32	111.62
13	A	813	CLA	O2A-C1-C2	-2.13	103.94	108.55
13	A	837	CLA	C2A-C1A-NA	-2.13	108.89	111.24
13	A	855	CLA	C2C-C1C-NC	-2.13	108.45	110.17
15	A	852	BCR	C20-C21-C22	-2.12	124.23	127.29
13	B	837	CLA	C4D-C3D-CAD	-2.12	105.45	108.05
15	F	1302	BCR	C37-C22-C21	-2.12	119.91	122.92
13	B	805	CLA	C11-C10-C8	-2.12	109.03	115.14
13	B	824	CLA	OBD-CAD-C3D	-2.12	123.97	127.91
13	B	801	CLA	C11-C10-C8	-2.12	109.04	115.14
14	A	846	PQN	C14-C13-C12	-2.12	119.33	123.52
13	B	836	CLA	C11-C10-C8	-2.12	109.05	115.14
14	B	840	PQN	C2M-C2-C3	-2.11	120.00	124.20
13	A	801	CLA	CMB-C2B-C1B	-2.11	125.37	128.62
13	B	835	CLA	C1D-CHD-C4C	2.11	125.87	122.60
13	A	842	CLA	C1-O2A-CGA	2.11	122.89	116.98
13	A	823	CLA	C2A-C3A-C4A	2.11	104.65	101.40
13	A	825	CLA	C1-O2A-CGA	2.11	122.89	116.98
13	B	819	CLA	C4B-CHC-C1C	-2.11	124.69	127.47
13	A	808	CLA	C2A-C3A-C4A	2.11	104.64	101.40
13	B	824	CLA	C1-C2-C3	-2.11	122.44	126.19
15	L	1005	BCR	C12-C13-C14	-2.11	115.73	118.97
13	A	811	CLA	C1D-CHD-C4C	2.11	125.87	122.60
13	A	823	CLA	CAA-CBA-CGA	-2.11	106.47	113.27
13	A	806	CLA	C11-C12-C13	-2.10	109.09	115.14
13	B	827	CLA	C4D-C3D-CAD	-2.10	105.47	108.05
15	A	850	BCR	C34-C9-C10	-2.10	119.94	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1201	CLA	C2A-C3A-C4A	2.10	104.63	101.40
15	F	1302	BCR	C4-C5-C6	-2.10	120.04	122.84
15	L	1006	BCR	C33-C5-C6	-2.10	122.13	124.51
15	F	1302	BCR	C16-C17-C18	-2.10	124.27	127.29
13	A	805	CLA	C1D-CHD-C4C	2.09	125.85	122.60
13	B	831	CLA	CED-O2D-CGD	-2.09	111.03	116.02
15	B	847	BCR	C15-C14-C13	-2.09	124.28	127.29
13	A	822	CLA	C2A-C1A-CHA	2.09	127.46	123.83
13	B	808	CLA	C2A-C3A-C4A	2.09	104.62	101.40
15	B	842	BCR	C2-C3-C4	2.09	116.81	111.48
13	B	821	CLA	C4D-C3D-CAD	-2.09	105.48	108.05
13	A	843	CLA	C11-C12-C13	-2.09	109.11	115.14
13	B	802	CLA	CGD-CBD-CAD	-2.09	103.85	110.96
13	B	828	CLA	CAA-C2A-C1A	2.09	116.85	111.62
13	A	826	CLA	C2A-C1A-CHA	2.09	127.45	123.83
13	A	828	CLA	C11-C10-C8	-2.09	109.12	115.14
15	I	102	BCR	C19-C18-C17	-2.09	115.76	118.97
13	B	819	CLA	C2C-C1C-NC	-2.09	108.48	110.17
13	B	811	CLA	C2A-C1A-CHA	2.09	127.45	123.83
15	A	849	BCR	C4-C5-C6	-2.09	120.06	122.84
13	B	801	CLA	C4B-CHC-C1C	-2.09	124.72	127.47
13	B	836	CLA	CAA-C2A-C1A	2.09	116.83	111.62
13	M	1202	CLA	CAA-C2A-C1A	2.09	116.83	111.62
15	B	849	BCR	C21-C20-C19	-2.09	116.20	123.24
15	A	847	BCR	C30-C25-C26	-2.08	119.58	122.60
13	A	828	CLA	C4-C3-C2	-2.08	119.39	123.52
13	A	813	CLA	C2A-C3A-C4A	2.08	104.61	101.40
15	A	849	BCR	C34-C9-C10	-2.08	119.96	122.92
13	A	814	CLA	OBD-CAD-C3D	-2.08	124.03	127.91
13	A	825	CLA	C3B-CAB-CBB	-2.08	121.64	125.95
13	B	807	CLA	CBD-CHA-C1A	-2.08	126.05	128.77
13	A	837	CLA	CHA-C1A-NA	-2.08	121.94	126.22
15	B	841	BCR	C15-C16-C17	-2.08	118.75	123.36
15	B	845	BCR	C19-C18-C17	-2.08	115.77	118.97
13	I	101	CLA	C11-C12-C13	-2.08	109.15	115.14
13	B	801	CLA	C1D-CHD-C4C	2.08	125.82	122.60
13	A	831	CLA	C1D-CHD-C4C	2.08	125.82	122.60
15	F	1302	BCR	C8-C7-C6	-2.08	121.19	127.32
13	A	841	CLA	C2A-C3A-C4A	2.08	104.59	101.40
13	A	845	CLA	C2A-C3A-C4A	2.07	104.59	101.40
13	A	832	CLA	O2D-CGD-O1D	-2.07	119.58	123.79
13	A	817	CLA	C1D-CHD-C4C	2.08	125.82	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	834	CLA	C4B-CHC-C1C	-2.07	124.74	127.47
13	A	833	CLA	CBD-CHA-C1A	2.07	131.48	128.77
13	A	810	CLA	C1D-CHD-C4C	2.07	125.81	122.60
13	A	801	CLA	C2C-C1C-NC	-2.07	108.49	110.17
13	A	813	CLA	C6-C7-C8	-2.07	109.17	115.14
15	A	849	BCR	C21-C20-C19	-2.07	116.25	123.24
15	A	850	BCR	C31-C1-C6	-2.07	106.90	110.33
15	B	846	BCR	C15-C16-C17	-2.07	118.78	123.36
13	B	805	CLA	C2C-C1C-NC	-2.07	108.49	110.17
13	B	804	CLA	C4-C3-C2	-2.07	119.42	123.52
15	I	102	BCR	C2-C3-C4	2.07	116.75	111.48
13	A	830	CLA	C11-C10-C8	-2.07	109.19	115.14
13	A	834	CLA	C11-C10-C8	-2.06	109.19	115.14
13	A	824	CLA	CAD-CBD-CHA	-2.07	97.15	103.30
13	L	1004	CLA	C4D-C3D-CAD	-2.06	105.51	108.05
13	A	833	CLA	CMD-C2D-C3D	2.07	128.22	124.97
15	B	842	BCR	C27-C26-C25	-2.06	120.09	122.84
15	J	1105	BCR	C12-C13-C14	-2.06	115.80	118.97
13	B	826	CLA	C1D-CHD-C4C	2.06	125.80	122.60
13	B	808	CLA	C2C-C1C-NC	-2.06	108.50	110.17
13	A	831	CLA	C2C-C1C-NC	-2.06	108.50	110.17
13	B	834	CLA	C3B-CAB-CBB	-2.06	121.69	125.95
13	A	810	CLA	C2C-C1C-NC	-2.06	108.50	110.17
13	A	812	CLA	C1-O2A-CGA	2.06	122.74	116.98
13	B	835	CLA	C3B-CAB-CBB	-2.05	121.70	125.95
13	A	803	CLA	C2A-C3A-C4A	2.05	104.56	101.40
15	I	102	BCR	C31-C1-C6	-2.05	106.93	110.33
13	B	812	CLA	O2D-CGD-O1D	-2.05	119.62	123.79
13	A	810	CLA	C4B-CHC-C1C	-2.05	124.77	127.47
13	B	824	CLA	C2A-C3A-C4A	2.05	104.56	101.40
13	B	815	CLA	O2D-CGD-O1D	-2.05	119.62	123.79
13	A	834	CLA	CGD-CBD-CHA	2.05	117.93	110.96
13	B	815	CLA	O2A-C1-C2	-2.05	104.11	108.55
13	I	101	CLA	O2A-CGA-CBA	2.05	118.39	111.94
15	A	851	BCR	C4-C5-C6	-2.05	120.11	122.84
13	A	820	CLA	C11-C10-C8	-2.05	109.24	115.14
13	B	803	CLA	CAD-CBD-CHA	-2.05	97.21	103.30
13	J	1101	CLA	C11-C12-C13	-2.05	109.24	115.14
13	B	823	CLA	C2A-C1A-CHA	2.05	127.38	123.83
13	B	822	CLA	C4-C3-C2	-2.05	119.47	123.52
13	A	842	CLA	C1D-CHD-C4C	2.05	125.77	122.60
13	B	812	CLA	O2A-C1-C2	-2.04	104.12	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	1302	BCR	C21-C20-C19	-2.04	116.34	123.24
13	B	806	CLA	CAA-C2A-C3A	2.04	117.87	113.04
13	A	830	CLA	O2A-CGA-CBA	2.04	118.37	111.94
13	L	1002	CLA	O2A-CGA-CBA	2.04	118.37	111.94
13	B	812	CLA	C2C-C1C-NC	-2.04	108.52	110.17
15	B	843	BCR	C15-C16-C17	-2.04	118.84	123.36
13	B	820	CLA	CED-O2D-CGD	2.04	120.87	116.02
13	B	822	CLA	C5-C6-C7	-2.04	109.42	113.25
15	B	845	BCR	C11-C10-C9	-2.04	124.35	127.29
13	B	818	CLA	C2A-C3A-C4A	2.04	104.54	101.40
15	J	1105	BCR	C39-C30-C25	-2.04	106.95	110.33
13	B	835	CLA	CHA-C1A-NA	-2.04	122.04	126.22
13	B	827	CLA	O2A-CGA-CBA	2.04	118.35	111.94
13	A	813	CLA	CMD-C2D-C3D	2.04	128.18	124.97
13	B	811	CLA	C4-C3-C5	2.04	118.48	115.39
13	B	826	CLA	C6-C7-C8	-2.04	109.27	115.14
15	B	847	BCR	C21-C20-C19	-2.04	116.37	123.24
13	A	805	CLA	CAA-C2A-C1A	2.03	116.70	111.62
13	B	823	CLA	C4D-C3D-CAD	-2.03	105.55	108.05
13	A	827	CLA	O2D-CGD-O1D	-2.03	119.66	123.79
15	A	849	BCR	C20-C19-C18	-2.03	120.58	126.38
13	B	802	CLA	C11-C10-C8	-2.03	109.29	115.14
15	J	1104	BCR	C36-C18-C17	-2.03	120.04	122.92
13	B	825	CLA	CAA-C2A-C1A	2.03	116.68	111.62
13	A	822	CLA	C1D-CHD-C4C	2.03	125.74	122.60
13	A	842	CLA	C4B-CHC-C1C	-2.03	124.80	127.47
15	B	844	BCR	C20-C21-C22	-2.03	124.37	127.29
13	A	830	CLA	C1D-CHD-C4C	2.03	125.74	122.60
13	A	828	CLA	C2A-C3A-C4A	2.03	104.52	101.40
13	J	1101	CLA	C4D-C3D-CAD	-2.03	105.56	108.05
15	L	1006	BCR	C23-C24-C25	-2.03	121.34	127.32
13	B	838	CLA	CMD-C2D-C3D	2.02	128.16	124.97
13	A	825	CLA	CAA-CBA-CGA	-2.02	106.74	113.27
13	M	1201	CLA	C2C-C1C-NC	-2.02	108.53	110.17
13	B	831	CLA	C11-C10-C8	-2.02	109.32	115.14
15	F	1302	BCR	C1-C6-C7	2.02	121.29	115.69
13	B	839	CLA	C4B-CHC-C1C	-2.02	124.81	127.47
13	B	833	CLA	C2A-C3A-C4A	2.02	104.51	101.40
15	A	847	BCR	C16-C15-C14	-2.02	118.89	123.36
15	B	850	BCR	C16-C15-C14	-2.02	118.89	123.36
13	I	101	CLA	C4-C3-C2	-2.02	119.53	123.52
15	B	849	BCR	C23-C22-C21	-2.02	115.87	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	814	CLA	C2A-C3A-C4A	2.01	104.50	101.40
15	B	850	BCR	C40-C30-C25	-2.02	106.99	110.33
15	B	847	BCR	C35-C13-C14	-2.01	120.06	122.92
13	B	837	CLA	C3B-CAB-CBB	-2.01	121.78	125.95
13	B	827	CLA	C7-C6-C5	-2.01	107.08	113.01
13	A	836	CLA	C2C-C1C-NC	-2.01	108.54	110.17
13	B	805	CLA	C2A-C3A-C4A	2.01	104.49	101.40
13	M	1202	CLA	C2C-C1C-NC	-2.01	108.54	110.17
13	A	826	CLA	CAA-C2A-C1A	2.01	116.64	111.62
15	A	847	BCR	C1-C6-C5	-2.01	119.69	122.60
13	A	806	CLA	CBD-CHA-C1A	2.01	131.40	128.77
13	B	831	CLA	C2A-C3A-C4A	2.01	104.49	101.40
15	J	1104	BCR	C1-C6-C5	-2.01	119.69	122.60
13	B	838	CLA	C4-C3-C2	-2.01	119.54	123.52
13	B	805	CLA	C11-C12-C13	-2.01	109.36	115.14
13	A	844	CLA	C2A-C3A-C4A	2.01	104.49	101.40
13	B	829	CLA	C4B-CHC-C1C	-2.01	124.83	127.47
15	A	852	BCR	C34-C9-C10	-2.01	120.07	122.92
13	A	819	CLA	C7-C6-C5	-2.00	107.11	113.01
13	A	825	CLA	C2C-C1C-NC	-2.00	108.55	110.17
13	A	825	CLA	C4D-C3D-CAD	-2.00	105.59	108.05
13	B	831	CLA	CMD-C2D-C3D	2.00	128.12	124.97
13	A	823	CLA	O2A-CGA-CBA	2.00	118.23	111.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/755 (98%)	1.27	140 (18%) 2 4	42, 99, 157, 202	0
2	B	739/740 (99%)	1.09	106 (14%) 3 7	34, 76, 126, 215	0
3	C	80/80 (100%)	0.92	4 (5%) 28 27	46, 72, 126, 138	0
4	D	138/138 (100%)	1.51	37 (26%) 1 4	45, 72, 117, 137	0
5	E	69/75 (92%)	1.83	26 (37%) 1 2	77, 100, 148, 194	0
6	F	141/164 (85%)	1.04	16 (11%) 6 11	54, 83, 136, 158	0
7	I	38/38 (100%)	1.11	6 (15%) 3 6	10, 36, 74, 78	0
8	J	41/41 (100%)	1.15	4 (9%) 8 13	65, 89, 136, 165	0
9	K	46/83 (55%)	1.73	13 (28%) 1 3	55, 87, 141, 169	0
10	L	151/154 (98%)	0.79	8 (5%) 25 26	14, 49, 104, 140	0
11	M	31/31 (100%)	0.95	2 (6%) 18 22	31, 51, 80, 92	0
12	X	29/35 (82%)	1.04	5 (17%) 2 5	59, 80, 120, 155	0
All	All	2243/2334 (96%)	1.18	367 (16%) 2 6	10, 81, 141, 215	0

All (367) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	52	ALA	5.8
9	K	31	ARG	5.5
1	A	244	LEU	5.3
1	A	207	LEU	5.0
1	A	210	LEU	4.8
1	A	268	PHE	4.7
2	B	497	ASN	4.6
1	A	34	PHE	4.6
2	B	309	PHE	4.5
2	B	226	THR	4.5
9	K	32	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	168	MET	4.3
3	C	80	TYR	4.3
1	A	33	HIS	4.3
4	D	83	TYR	4.3
2	B	225	PHE	4.2
12	X	12	ARG	4.2
1	A	40	ARG	4.2
2	B	229	TRP	4.1
4	D	29	ILE	4.1
1	A	260	PHE	4.1
1	A	321	ILE	4.1
9	K	66	GLY	4.0
1	A	13	ARG	4.0
1	A	218	HIS	4.0
1	A	211	ALA	4.0
4	D	28	ALA	3.9
4	D	27	TYR	3.9
9	K	34	ILE	3.8
10	L	146	ASP	3.8
1	A	267	PHE	3.8
1	A	204	LEU	3.8
1	A	502	ALA	3.8
1	A	243	ILE	3.7
1	A	55	ALA	3.7
9	K	65	PHE	3.7
1	A	237	PRO	3.7
2	B	87	ALA	3.7
2	B	312	THR	3.7
1	A	92	PHE	3.6
12	X	35	ALA	3.6
1	A	523	LYS	3.6
2	B	291	ARG	3.6
1	A	172	MET	3.6
2	B	397	LEU	3.6
4	D	55	LEU	3.6
4	D	57	TYR	3.6
1	A	501	THR	3.6
2	B	703	PRO	3.6
1	A	259	GLY	3.6
5	E	2	GLN	3.5
1	A	24	SER	3.5
2	B	495	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	500	GLY	3.5
8	J	26	LEU	3.4
2	B	313	LYS	3.4
1	A	241	GLU	3.4
1	A	309	ILE	3.4
2	B	90	ILE	3.4
1	A	624	THR	3.4
1	A	15	VAL	3.4
1	A	515	GLY	3.4
1	A	289	THR	3.4
2	B	496	GLY	3.3
9	K	41	PRO	3.3
2	B	343	CYS	3.3
1	A	80	LEU	3.3
1	A	734	HIS	3.3
1	A	160	CYS	3.3
6	F	95	ASN	3.3
8	J	33	TYR	3.3
1	A	261	PHE	3.3
1	A	315	TYR	3.3
2	B	552	LEU	3.2
5	E	1	VAL	3.2
1	A	303	ALA	3.2
2	B	181	LEU	3.2
8	J	25	ILE	3.2
5	E	53	SER	3.2
1	A	60	THR	3.2
5	E	54	GLY	3.2
1	A	516	ASP	3.1
4	D	25	GLU	3.1
1	A	54	LEU	3.1
1	A	205	LEU	3.1
10	L	149	MET	3.1
1	A	159	TYR	3.1
2	B	280	ALA	3.1
4	D	94	ILE	3.1
2	B	609	GLU	3.1
1	A	305	ALA	3.1
1	A	377	MET	3.1
4	D	2	THR	3.1
1	A	322	GLY	3.1
1	A	499	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	79	HIS	3.0
4	D	84	ARG	3.0
5	E	67	GLU	3.0
4	D	18	LEU	3.0
5	E	6	LYS	3.0
1	A	320	GLY	3.0
1	A	522	GLY	3.0
2	B	227	GLY	3.0
1	A	206	GLY	3.0
1	A	503	PRO	3.0
1	A	527	MET	3.0
1	A	171	LEU	2.9
2	B	574	CYS	2.9
12	X	9	TYR	2.9
5	E	5	SER	2.9
1	A	25	PHE	2.9
1	A	623	GLY	2.9
2	B	283	PHE	2.9
12	X	8	THR	2.9
7	I	1	MET	2.9
1	A	152	ILE	2.9
1	A	302	LEU	2.9
2	B	517	THR	2.9
2	B	187	LEU	2.9
2	B	489	SER	2.9
4	D	54	ASN	2.9
1	A	208	GLY	2.9
2	B	407	LYS	2.9
1	A	175	ALA	2.8
2	B	492	TRP	2.8
4	D	46	ALA	2.8
1	A	630	THR	2.8
9	K	64	SER	2.8
1	A	22	PRO	2.8
2	B	228	ASN	2.8
1	A	373	HIS	2.8
4	D	80	TYR	2.8
1	A	234	LYS	2.8
2	B	494	ASN	2.8
4	D	49	MET	2.8
7	I	35	GLU	2.8
2	B	568	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	328	THR	2.7
3	C	7	TYR	2.7
9	K	30	GLY	2.7
1	A	150	SER	2.7
4	D	1	THR	2.7
1	A	493	LEU	2.7
5	E	22	THR	2.7
5	E	4	GLY	2.7
2	B	186	SER	2.7
2	B	277	LEU	2.7
2	B	499	TRP	2.7
1	A	366	LEU	2.7
2	B	224	PHE	2.7
2	B	296	ILE	2.7
2	B	340	HIS	2.7
6	F	136	ILE	2.7
2	B	78	GLN	2.7
1	A	509	ALA	2.7
4	D	129	LYS	2.7
1	A	21	VAL	2.7
1	A	156	PHE	2.7
2	B	490	THR	2.6
1	A	32	GLY	2.6
1	A	521	GLY	2.6
2	B	491	ALA	2.6
2	B	103	PHE	2.6
9	K	35	GLN	2.6
5	E	33	LYS	2.6
5	E	46	THR	2.6
5	E	38	VAL	2.6
2	B	274	HIS	2.6
2	B	97	LYS	2.6
2	B	508	ASN	2.6
1	A	94	GLY	2.6
4	D	56	VAL	2.6
1	A	526	MET	2.6
1	A	310	ILE	2.6
1	A	151	GLY	2.6
2	B	488	ALA	2.6
2	B	176	HIS	2.6
2	B	178	LEU	2.6
1	A	304	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	123	PRO	2.6
5	E	23	VAL	2.5
1	A	180	TYR	2.5
10	L	148	ILE	2.5
6	F	141	ARG	2.5
2	B	473	LEU	2.5
2	B	614	GLN	2.5
1	A	307	LEU	2.5
2	B	481	LEU	2.5
4	D	26	LYS	2.5
1	A	625	VAL	2.5
2	B	548	ARG	2.5
1	A	223	ILE	2.5
2	B	179	ALA	2.5
4	D	130	PHE	2.5
1	A	56	HIS	2.5
2	B	424	HIS	2.5
2	B	86	ILE	2.5
2	B	320	MET	2.5
1	A	711	LEU	2.5
10	L	150	THR	2.5
6	F	64	LEU	2.5
8	J	41	LEU	2.5
2	B	105	GLN	2.5
1	A	403	PHE	2.5
1	A	634	ILE	2.5
4	D	133	LYS	2.4
1	A	692	SER	2.4
2	B	36	MET	2.4
4	D	50	ARG	2.4
2	B	472	LYS	2.4
5	E	17	TYR	2.4
1	A	119	PRO	2.4
1	A	318	ASN	2.4
1	A	755	GLY	2.4
4	D	3	LEU	2.4
1	A	306	VAL	2.4
4	D	92	VAL	2.4
1	A	19	ASP	2.4
9	K	55	GLY	2.4
2	B	281	VAL	2.4
2	B	212	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	240	HIS	2.4
1	A	376	ALA	2.4
1	A	203	GLY	2.4
4	D	128	LEU	2.4
5	E	36	VAL	2.4
7	I	2	MET	2.4
1	A	319	TRP	2.4
1	A	519	ALA	2.4
2	B	241	HIS	2.4
1	A	314	MET	2.4
1	A	183	ARG	2.4
1	A	246	PRO	2.4
1	A	279	LEU	2.4
3	C	58	PRO	2.4
2	B	26	MET	2.4
4	D	31	TRP	2.4
1	A	16	VAL	2.3
2	B	361	TYR	2.3
5	E	37	ILE	2.3
1	A	642	SER	2.3
2	B	185	SER	2.3
6	F	26	ALA	2.3
2	B	1	ALA	2.3
10	L	143	LEU	2.3
1	A	23	THR	2.3
2	B	672	SER	2.3
1	A	61	HIS	2.3
1	A	202	ALA	2.3
1	A	737	LEU	2.3
1	A	78	GLY	2.3
1	A	182	LYS	2.3
2	B	441	VAL	2.3
2	B	617	GLU	2.3
5	E	51	SER	2.3
9	K	22	CYS	2.3
1	A	132	GLY	2.3
10	L	140	GLU	2.3
5	E	26	VAL	2.3
11	M	31	LYS	2.3
2	B	713	LEU	2.3
1	A	557	VAL	2.3
2	B	605	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	113	ASP	2.3
6	F	56	ARG	2.3
1	A	28	TRP	2.3
2	B	314	VAL	2.3
1	A	317	THR	2.2
1	A	187	LEU	2.2
4	D	59	ALA	2.2
2	B	493	PRO	2.2
2	B	282	LEU	2.2
4	D	60	ARG	2.2
1	A	626	ALA	2.2
2	B	35	GLY	2.2
4	D	93	LEU	2.2
6	F	111	LEU	2.2
1	A	270	PHE	2.2
4	D	47	ALA	2.2
2	B	510	GLY	2.2
2	B	232	TYR	2.2
1	A	51	LEU	2.2
2	B	649	LEU	2.2
2	B	646	THR	2.2
6	F	131	ALA	2.2
1	A	631	VAL	2.2
1	A	413	ALA	2.2
2	B	344	LEU	2.2
3	C	46	ASP	2.2
7	I	9	PHE	2.2
2	B	420	ALA	2.2
1	A	378	PRO	2.2
2	B	19	ARG	2.2
2	B	81	VAL	2.2
1	A	520	VAL	2.2
2	B	23	ALA	2.2
5	E	42	LYS	2.2
11	M	3	LEU	2.2
1	A	508	THR	2.2
2	B	699	TRP	2.2
5	E	31	GLY	2.2
1	A	164	GLY	2.2
2	B	712	ARG	2.2
1	A	675	LEU	2.2
1	A	214	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	22	TYR	2.2
1	A	227	LEU	2.1
2	B	360	PRO	2.1
2	B	689	GLU	2.1
7	I	12	TRP	2.1
2	B	643	PRO	2.1
4	D	53	GLU	2.1
6	F	135	GLU	2.1
5	E	50	GLY	2.1
6	F	94	ALA	2.1
2	B	310	PHE	2.1
1	A	374	MET	2.1
6	F	63	PHE	2.1
2	B	21	TRP	2.1
2	B	96	GLY	2.1
6	F	55	GLY	2.1
1	A	627	PRO	2.1
1	A	85	ILE	2.1
1	A	287	PRO	2.1
1	A	313	HIS	2.1
2	B	696	LEU	2.1
6	F	129	LEU	2.1
4	D	41	MET	2.1
10	L	107	SER	2.1
1	A	59	ASP	2.1
1	A	91	TYR	2.1
2	B	3	LYS	2.1
1	A	238	LEU	2.1
2	B	355	MET	2.1
6	F	20	ALA	2.1
1	A	517	VAL	2.1
2	B	498	VAL	2.1
4	D	81	LYS	2.1
2	B	91	TRP	2.1
1	A	618	GLN	2.1
4	D	78	ASN	2.1
10	L	73	VAL	2.1
2	B	575	ASP	2.0
2	B	293	GLN	2.0
2	B	652	TRP	2.0
5	E	63	HIS	2.0
1	A	31	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	84	PHE	2.0
2	B	311	GLY	2.0
5	E	27	ASP	2.0
1	A	14	VAL	2.0
1	A	641	GLN	2.0
2	B	611	ASN	2.0
5	E	45	TYR	2.0
4	D	30	THR	2.0
1	A	558	LEU	2.0
7	I	3	GLY	2.0
2	B	327	GLU	2.0
4	D	21	ALA	2.0
6	F	108	LYS	2.0
9	K	23	ASN	2.0
2	B	275	HIS	2.0
6	F	69	LEU	2.0
5	E	19	GLU	2.0
12	X	15	TRP	2.0
2	B	11	LEU	2.0
9	K	37	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
13	CLA	A	824	59/65	0.72	8.01	59,101,164,321	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	BCR	B	844	25/40	0.79	7.34	65,68,113,118	0
15	BCR	A	850	40/40	1.12	6.23	56,96,126,139	0
15	BCR	B	849	40/40	0.68	5.30	12,43,147,152	0
15	BCR	J	1104	40/40	1.38	5.27	64,78,113,120	0
15	BCR	B	846	40/40	1.10	4.61	75,91,131,137	0
15	BCR	A	852	40/40	1.11	4.45	78,107,149,162	0
15	BCR	J	1105	40/40	0.97	4.44	63,67,71,71	0
13	CLA	M	1202	45/65	0.94	4.44	51,149,183,198	0
15	BCR	B	847	40/40	0.72	4.16	40,51,116,126	0
15	BCR	B	843	40/40	0.90	4.09	45,59,82,86	0
15	BCR	A	849	40/40	1.65	4.05	95,136,179,183	0
15	BCR	F	1302	40/40	1.09	3.81	70,94,125,128	0
13	CLA	B	830	65/65	0.99	3.81	82,91,129,139	0
15	BCR	B	841	40/40	1.20	3.55	65,105,151,155	0
13	CLA	A	809	65/65	0.92	3.51	78,117,148,152	0
15	BCR	A	851	40/40	0.91	3.41	50,58,118,132	0
15	BCR	A	847	40/40	1.64	3.36	98,140,151,162	0
13	CLA	A	843	65/65	0.68	3.33	56,83,169,197	0
16	LHG	A	853	49/49	0.97	3.14	57,74,107,127	0
13	CLA	B	824	65/65	0.74	3.13	58,65,88,96	0
13	CLA	A	820	61/65	1.38	3.08	119,135,166,198	0
15	BCR	A	848	40/40	1.63	3.08	112,132,147,157	0
13	CLA	A	855	45/65	0.76	2.95	95,118,140,153	0
13	CLA	J	1101	65/65	0.87	2.93	77,129,178,357	0
13	CLA	B	818	47/65	0.84	2.91	56,99,146,292	0
15	BCR	B	850	40/40	0.88	2.90	83,107,144,146	0
13	CLA	A	826	65/65	0.69	2.85	53,80,112,127	0
15	BCR	M	1203	40/40	0.69	2.78	43,48,87,92	0
14	PQN	A	846	33/33	0.83	2.70	55,64,82,82	0
13	CLA	A	842	65/65	0.92	2.70	62,82,149,162	0
13	CLA	B	814	55/65	1.13	2.52	77,122,182,325	0
14	PQN	B	840	33/33	0.81	2.42	56,84,105,121	0
13	CLA	A	815	45/65	1.32	2.41	111,150,177,185	0
13	CLA	A	806	65/65	0.85	2.39	63,80,155,164	0
13	CLA	A	833	65/65	0.76	2.38	39,45,110,121	0
13	CLA	A	816	49/65	1.32	2.34	119,163,187,193	0
13	CLA	A	803	65/65	0.74	2.33	76,100,142,222	0
13	CLA	A	807	51/65	0.98	2.29	87,100,151,177	0
13	CLA	A	808	65/65	0.63	2.22	72,89,172,177	0
15	BCR	I	102	40/40	0.50	2.18	19,20,48,52	0
13	CLA	A	827	65/65	0.90	2.18	68,103,137,248	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
13	CLA	A	829	65/65	0.88	2.18	83,108,179,197	0
13	CLA	A	834	65/65	0.63	2.15	39,40,92,96	0
15	BCR	B	842	40/40	0.93	2.13	48,76,129,134	0
18	LMG	B	848	55/55	0.72	2.13	42,51,67,114	0
13	CLA	B	804	65/65	0.74	2.05	45,51,117,199	0
13	CLA	B	839	65/65	0.57	2.00	35,49,151,215	0
15	BCR	B	845	40/40	0.77	2.00	60,66,78,82	0
13	CLA	B	811	65/65	0.79	1.97	48,71,108,145	0
15	BCR	L	1006	40/40	0.39	1.96	16,24,64,78	0
13	CLA	B	822	54/65	0.78	1.93	61,86,118,158	0
13	CLA	A	823	51/65	0.65	1.92	74,129,153,156	0
13	CLA	A	828	65/65	0.68	1.92	59,74,127,289	0
13	CLA	F	1301	45/65	0.88	1.89	94,137,167,175	0
13	CLA	B	815	59/65	0.76	1.89	55,58,76,293	0
13	CLA	B	835	60/65	0.51	1.84	65,106,240,292	0
13	CLA	B	838	65/65	0.75	1.84	35,45,102,125	0
13	CLA	B	816	60/65	0.86	1.83	46,53,111,221	0
13	CLA	B	813	45/65	0.84	1.82	51,86,132,141	0
13	CLA	L	1002	65/65	0.49	1.82	29,65,103,148	0
13	CLA	B	817	65/65	0.81	1.80	57,65,113,125	0
13	CLA	A	821	65/65	0.82	1.77	72,100,164,266	0
13	CLA	A	832	65/65	0.56	1.74	42,45,81,134	0
13	CLA	A	838	65/65	0.52	1.74	45,81,109,114	0
13	CLA	B	812	65/65	0.62	1.73	37,42,111,117	0
13	CLA	A	805	65/65	0.83	1.70	85,98,117,126	0
13	CLA	B	823	46/65	0.52	1.69	59,68,120,137	0
13	CLA	B	802	65/65	0.57	1.64	61,82,112,165	0
13	CLA	B	831	58/65	0.77	1.64	80,101,148,333	0
13	CLA	A	812	54/65	1.05	1.62	136,181,240,396	0
13	CLA	A	819	65/65	0.88	1.60	97,140,181,328	0
13	CLA	A	845	52/65	0.55	1.55	56,78,188,214	0
13	CLA	B	803	65/65	0.61	1.54	40,68,95,180	0
13	CLA	A	844	41/65	1.11	1.53	116,136,148,281	0
13	CLA	A	840	65/65	0.68	1.51	77,87,117,198	0
13	CLA	B	836	65/65	0.66	1.49	69,98,146,234	0
13	CLA	B	826	65/65	0.68	1.49	42,47,127,149	0
13	CLA	B	819	45/65	0.69	1.48	98,131,171,173	0
13	CLA	B	809	45/65	0.50	1.47	39,95,125,308	0
13	CLA	A	813	60/65	0.89	1.46	115,146,178,366	0
15	BCR	L	1005	40/40	0.59	1.44	11,16,81,93	0
13	CLA	L	1003	65/65	0.55	1.42	16,52,179,216	0
13	CLA	A	830	65/65	0.74	1.38	59,71,105,119	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
13	CLA	A	802	65/65	0.54	1.38	40,77,110,230	0
13	CLA	A	801	65/65	0.50	1.32	44,53,82,89	0
13	CLA	B	821	45/65	0.60	1.30	63,69,105,191	0
13	CLA	B	827	65/65	0.54	1.27	44,66,95,108	0
13	CLA	X	102	45/65	0.53	1.24	67,104,127,283	0
13	CLA	A	817	54/65	0.82	1.24	83,104,164,172	0
13	CLA	M	1201	54/65	0.59	1.22	34,42,121,127	0
13	CLA	A	837	51/65	0.49	1.14	52,56,96,147	0
13	CLA	L	1004	65/65	0.59	1.12	21,31,64,72	0
13	CLA	A	831	50/65	0.52	1.11	45,76,105,144	0
13	CLA	B	810	45/65	0.62	1.11	47,84,145,182	0
16	LHG	A	854	27/49	0.51	1.10	49,58,88,122	0
13	CLA	B	829	49/65	0.69	1.04	80,85,125,141	0
13	CLA	B	805	65/65	0.51	1.03	41,48,97,150	0
13	CLA	A	804	59/65	0.88	1.01	83,99,117,144	0
13	CLA	B	807	65/65	0.61	0.97	38,65,106,122	0
13	CLA	A	811	65/65	0.84	0.95	95,134,173,321	0
13	CLA	B	808	65/65	0.62	0.94	36,41,97,103	0
13	CLA	J	1103	37/65	0.66	0.94	85,117,155,158	0
13	CLA	B	825	65/65	0.44	0.93	40,60,136,157	0
13	CLA	J	1102	45/65	0.69	0.93	75,111,128,280	0
13	CLA	B	801	65/65	0.41	0.87	57,68,123,322	0
13	CLA	A	841	51/65	0.55	0.84	80,105,182,204	0
13	CLA	B	806	65/65	0.49	0.79	33,63,107,170	0
13	CLA	A	818	54/65	0.67	0.78	92,136,168,207	0
13	CLA	I	101	65/65	0.48	0.75	33,57,85,338	0
13	CLA	B	832	45/65	0.62	0.68	71,121,142,247	0
13	CLA	B	820	55/65	0.68	0.61	77,105,141,146	0
13	CLA	A	835	54/65	0.72	0.51	54,79,117,204	0
13	CLA	A	822	49/65	0.75	0.40	102,126,157,235	0
13	CLA	B	834	45/65	0.74	0.39	91,118,151,158	0
13	CLA	A	825	65/65	0.47	0.38	74,102,152,193	0
13	CLA	A	814	45/65	0.71	0.32	108,150,172,174	0
13	CLA	B	828	45/65	0.63	0.28	70,80,132,193	0
16	LHG	X	101	23/49	0.61	0.16	78,81,207,208	0
13	CLA	A	836	45/65	0.70	0.10	63,96,163,234	0
13	CLA	A	810	45/65	0.61	0.03	109,136,151,223	0
13	CLA	A	839	47/65	0.41	0.03	48,51,119,202	0
13	CLA	B	833	45/65	0.71	-0.00	77,104,141,148	0
13	CLA	B	837	47/65	0.46	-0.11	65,71,119,193	0
17	SF4	A	856	8/8	0.27	-1.28	49,50,150,174	0
17	SF4	C	101	8/8	0.23	-1.97	48,48,49,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	SF4	C	102	8/8	0.18	-2.11	47,48,122,359	0
19	CA	L	1001	1/1	0.18	-2.53	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.