



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:44 AM GMT

PDB ID : 1JB0
Title : Crystal Structure of Photosystem I: a Photosynthetic Reaction Center and Core Antenna System from Cyanobacteria
Authors : Jordan, P.; Fromme, P.; Witt, H.T.; Klukas, O.; Saenger, W.; Krauss, N.
Deposited on : 2001-06-01
Resolution : 2.50 Å(reported)

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

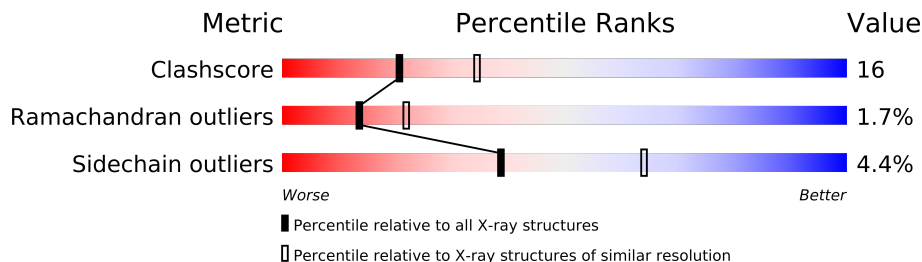
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	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	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 24198 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 1 REACTION CENTRE 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 1 REACTION CENTRE 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 1 REACTION CENTRE 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 1 REACTION CENTRE 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 1 REACTION CENTRE 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 1 REACTION CENTRE SUBUNIT X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O	S	0	0	0
			222	130	46	46				

- Molecule 10 is a protein called PHOTOSYSTEM 1 REACTION CENTRE 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 are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ARG	PRO	CONFLICT	UNP P25902
L	144	VAL	-	SEE REMARK 999	UNP P25902
L	145	VAL	-	SEE REMARK 999	UNP P25902
L	146	ASP	-	SEE REMARK 999	UNP P25902
L	147	GLY	-	SEE REMARK 999	UNP P25902
L	148	ILE	-	SEE REMARK 999	UNP P25902
L	149	MET	-	SEE REMARK 999	UNP P25902
L	150	THR	-	SEE REMARK 999	UNP P25902
L	151	GLY	-	SEE REMARK 999	UNP P25902
L	152	LEU	-	SEE REMARK 999	UNP P25902
L	153	PHE	-	SEE REMARK 999	UNP P25902
L	154	ASN	-	SEE REMARK 999	UNP P25902

- Molecule 11 is a protein called PHOTOSYSTEM 1 REACTION CENTRE 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			

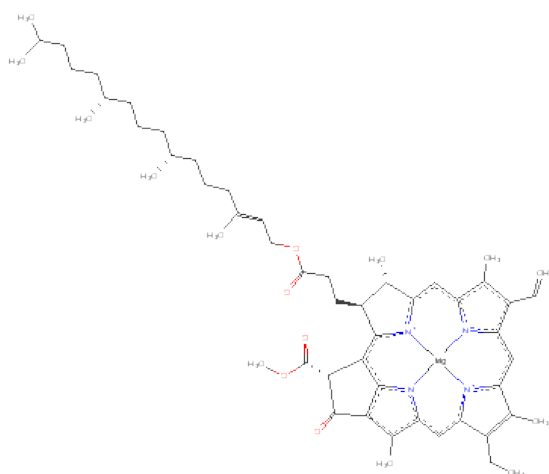
- Molecule 12 is a protein called PHOTOSYSTEM I SUBUNIT PSAX.

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

- Molecule 13 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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



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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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

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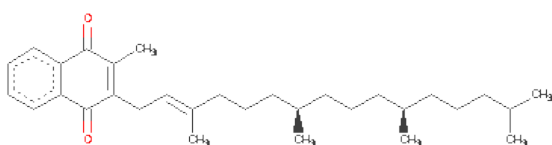
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5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

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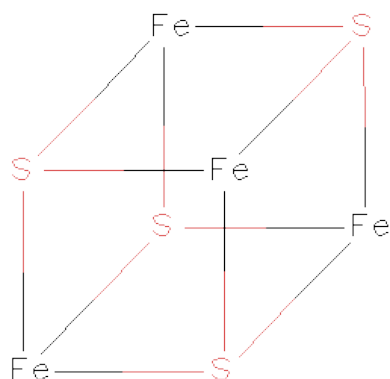
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	J	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
14	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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



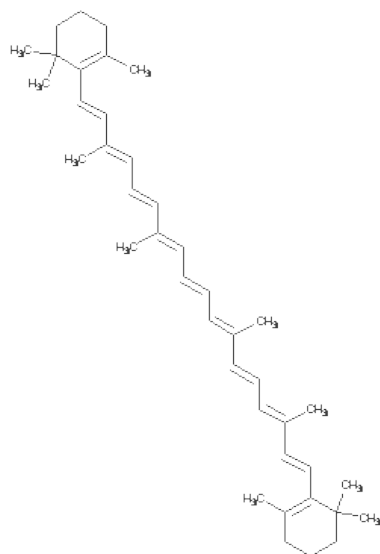
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			33	31	2		
15	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



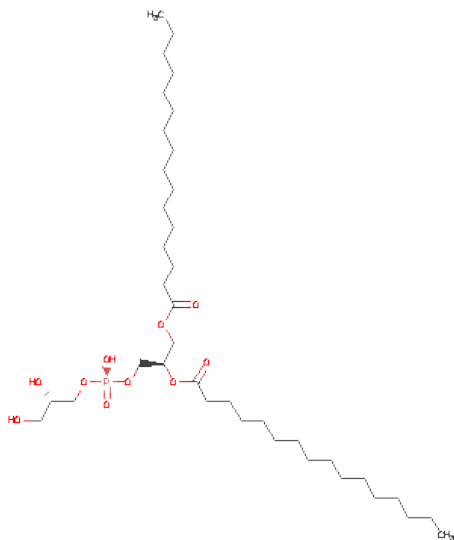
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	Fe	S	0	0
			8	4	4		
16	C	1	Total	Fe	S	0	0
			8	4	4		
16	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



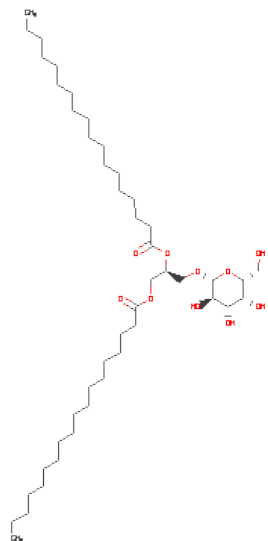
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	B	1	Total C 25 25	0	0
17	B	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	J	1	Total C 40 40	0	0
17	J	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	J	1	Total C 40 40	0	0
17	F	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	I	1	Total C 40 40	0	0
17	L	1	Total C 40 40	0	0
17	I	1	Total C 40 40	0	0
17	M	1	Total C 40 40	0	0
17	L	1	Total C 40 40	0	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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



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

- Molecule 20 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	53	Total	O		0	0
			53	53			
20	B	65	Total	O		0	0
			65	65			
20	C	21	Total	O		0	0
			21	21			
20	D	17	Total	O		0	0
			17	17			
20	E	5	Total	O		0	0
			5	5			
20	F	6	Total	O		0	0
			6	6			
20	I	3	Total	O		0	0
			3	3			
20	J	1	Total	O		0	0
			1	1			
20	L	27	Total	O		0	0
			27	27			
20	M	3	Total	O		0	0
			3	3			

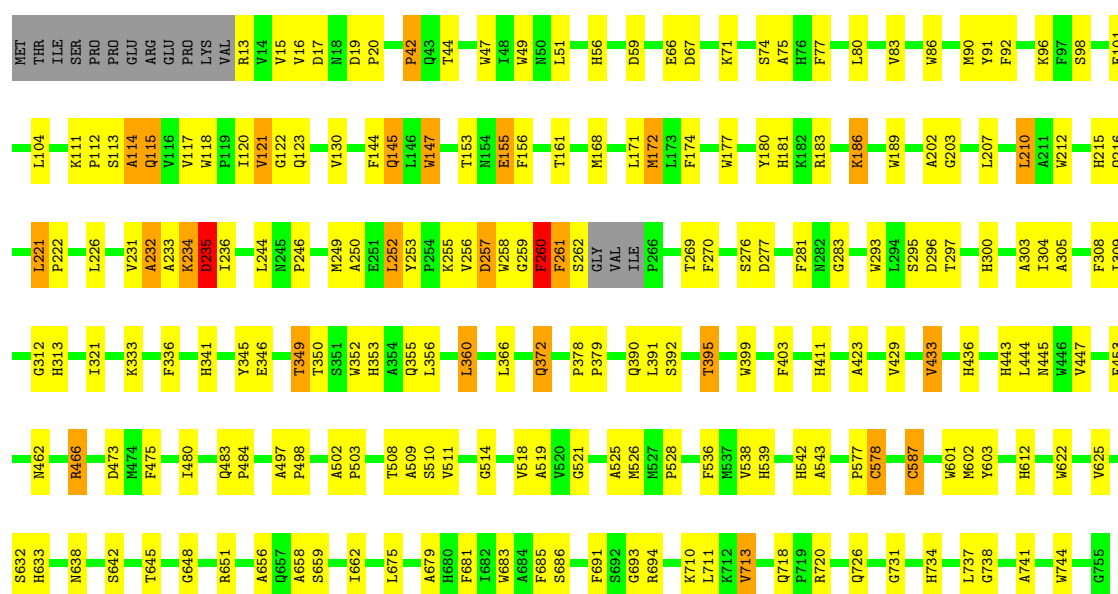
3 Residue-property plots

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

Note EDS was not executed.

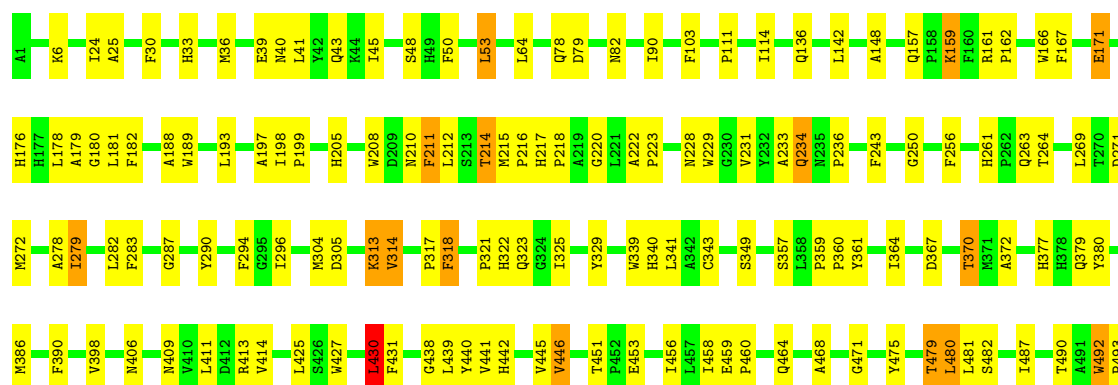
- Molecule 1: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1

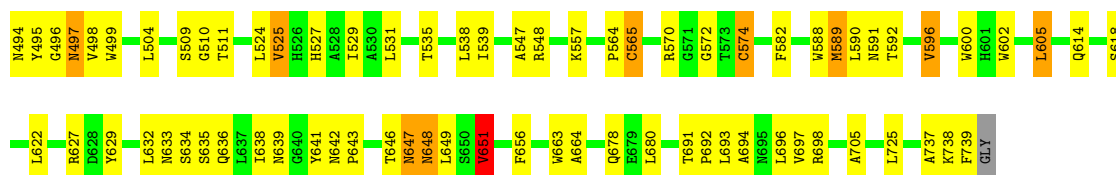
Chain A:



- Molecule 2: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

Chain B:





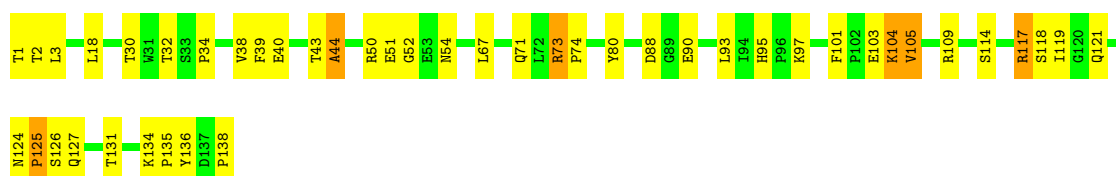
• Molecule 3: PHOTOSYSTEM I IRON-SULFUR CENTER

Chain C:



• Molecule 4: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II

Chain D:



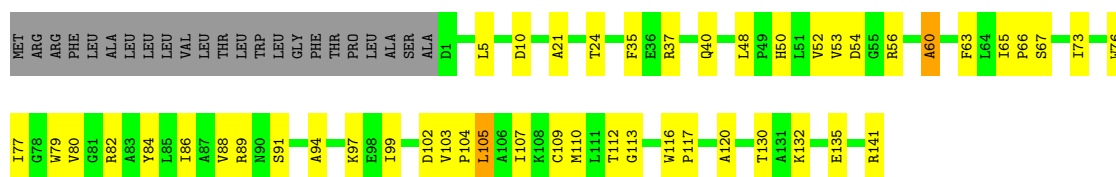
• Molecule 5: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV

Chain E:



• Molecule 6: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III

Chain F:



• Molecule 7: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII

Chain I:



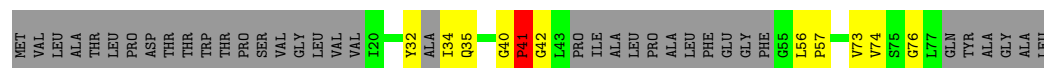
• Molecule 8: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX

Chain J:



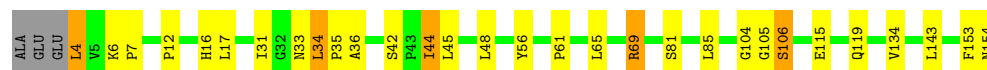
• Molecule 9: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X

Chain K: 



- Molecule 10: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI

Chain L: 



- Molecule 11: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII

Chain M: 



- Molecule 12: PHOTOSYSTEM I SUBUNIT PSAX

Chain X: 



4 Data and refinement statistics

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

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)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.3 (30.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.199 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24198	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.51	0/5983	0.66	2/8158 (0.0%)
2	B	0.56	0/6096	0.67	2/8332 (0.0%)
3	C	0.74	0/608	0.96	4/824 (0.5%)
4	D	0.57	0/1101	0.81	1/1492 (0.1%)
5	E	0.57	0/551	0.84	2/750 (0.3%)
6	F	0.47	0/1087	0.66	0/1476
7	I	0.66	0/312	0.75	0/425
8	J	0.45	0/350	0.65	0/477
9	K	0.52	0/219	0.86	3/297 (1.0%)
10	L	0.67	0/1148	0.75	0/1558
11	M	0.63	0/244	0.85	1/332 (0.3%)
12	X	0.55	0/242	0.67	0/332
All	All	0.55	0/17941	0.70	15/24453 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	80	TYR	CA-C-O	9.95	140.99	120.10
11	M	30	TYR	N-CA-C	7.84	132.18	111.00
4	D	131	THR	N-CA-C	-7.83	89.86	111.00
5	E	54	GLY	N-CA-C	7.52	131.91	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	GLY	N-CA-C	-6.39	97.13	113.10
3	C	60	ASP	CA-C-N	-6.29	103.37	117.20
9	K	57	PRO	N-CA-CB	6.14	110.67	103.30
3	C	60	ASP	C-N-CA	5.89	136.41	121.70
1	A	114	ALA	N-CA-C	-5.87	95.16	111.00
3	C	61	PHE	N-CA-CB	5.85	121.14	110.60
9	K	41	PRO	N-CA-CB	5.78	110.24	103.30
9	K	35	GLN	N-CA-C	5.35	125.45	111.00
2	B	430	LEU	CA-CB-CG	5.12	127.08	115.30
2	B	651	VAL	CB-CA-C	-5.10	101.72	111.40
5	E	55	VAL	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	61	PHE	Sidechain

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	5639	215	0
2	B	5879	0	5632	238	0
3	C	598	0	580	16	0
4	D	1075	0	1077	40	0
5	E	539	0	528	10	0
6	F	1065	0	1079	42	0
7	I	301	0	306	7	0
8	J	338	0	347	23	0
9	K	222	0	110	4	0
10	L	1119	0	1125	22	0
11	M	241	0	264	13	0
12	X	233	0	231	6	0
13	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	2687	0	2675	143	0
14	B	2349	0	2304	152	0
14	F	45	0	33	1	0
14	J	82	0	58	1	0
14	K	45	0	33	1	0
14	L	195	0	216	11	0
14	M	45	0	33	1	0
14	X	45	0	33	1	0
15	A	33	0	46	1	0
15	B	33	0	46	1	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
17	A	240	0	336	22	0
17	B	265	0	369	17	0
17	F	40	0	56	2	0
17	I	80	0	112	3	0
17	J	120	0	168	16	0
17	L	80	0	112	1	0
17	M	40	0	56	2	0
18	A	76	0	98	6	0
18	B	23	0	16	1	0
19	B	55	0	86	5	0
20	A	53	0	0	5	0
20	B	65	0	0	3	0
20	C	21	0	0	3	0
20	D	17	0	0	1	0
20	E	5	0	0	0	0
20	F	6	0	0	1	0
20	I	3	0	0	0	0
20	J	1	0	0	0	0
20	L	27	0	0	1	1
20	M	3	0	0	1	0
All	All	24198	0	23804	743	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 16.

All (743) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:J:31:ARG:HD3	17:J:4013:BCR:H312	1.25	1.17
2:B:622:LEU:HD12	14:B:1012:CLA:H11	1.29	1.15
1:A:508:THR:HG22	1:A:510:SER:H	1.18	1.07

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:159:LYS:H	2:B:159:LYS:HD2	1.18	1.05
4:D:50:ARG:H	4:D:54:ASN:HD21	1.06	1.01
2:B:243:PHE:H	2:B:263:GLN:HE22	1.07	1.01
2:B:231:VAL:O	2:B:234:GLN:HG2	1.63	0.99
2:B:406:ASN:HD22	2:B:409:ASN:HD21	0.98	0.96
1:A:536:PHE:HA	14:A:1136:CLA:HED1	1.45	0.96
2:B:494:ASN:HD22	2:B:496:GLY:H	1.13	0.93
11:M:31:LYS:O	11:M:31:LYS:HG2	1.70	0.92
1:A:353:HIS:HD2	1:A:411:HIS:HD1	1.21	0.88
4:D:117:ARG:HG3	4:D:121:GLN:HB2	1.54	0.88
17:A:4011:BCR:H362	14:B:1012:CLA:H42	1.55	0.87
1:A:117:VAL:HG13	1:A:123:GLN:HE21	1.42	0.84
2:B:406:ASN:ND2	2:B:409:ASN:HD21	1.76	0.83
8:J:24:GLY:HA3	14:J:1302:CLA:HBB1	1.60	0.83
4:D:101:PHE:HB2	4:D:104:LYS:HE2	1.59	0.83
8:J:31:ARG:HD3	17:J:4013:BCR:C31	2.08	0.83
1:A:333:LYS:O	14:A:1801:CLA:HBC3	1.81	0.81
2:B:509:SER:O	2:B:511:THR:N	2.12	0.81
1:A:203:GLY:HA2	14:A:1118:CLA:HBC1	1.63	0.80
1:A:391:LEU:O	1:A:395:THR:HG23	1.81	0.80
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.12	0.80
6:F:88:VAL:HG12	6:F:94:ALA:HA	1.63	0.79
6:F:88:VAL:HG11	6:F:97:LYS:HB2	1.64	0.79
2:B:494:ASN:ND2	2:B:496:GLY:H	1.80	0.78
1:A:345:TYR:O	1:A:349:THR:HB	1.84	0.78
2:B:459:GLU:HG3	6:F:5:LEU:HD11	1.63	0.78
2:B:243:PHE:H	2:B:263:GLN:NE2	1.82	0.78
1:A:508:THR:HG22	1:A:510:SER:N	1.96	0.77
2:B:313:LYS:O	2:B:314:VAL:HG22	1.85	0.77
3:C:37:GLN:NE2	4:D:105:VAL:HG22	1.99	0.77
2:B:278:ALA:HB2	14:B:1214:CLA:HBB1	1.66	0.77
2:B:339:TRP:HE1	14:B:1221:CLA:C2B	1.99	0.76
2:B:25:ALA:HB2	19:B:5002:LMG:H121	1.67	0.76
14:A:1011:CLA:HBB1	14:B:1012:CLA:HED1	1.67	0.75
1:A:231:VAL:O	1:A:232:ALA:HB3	1.87	0.75
14:A:1126:CLA:H192	17:J:4012:BCR:H14C	1.69	0.75
2:B:367:ASP:CG	2:B:370:THR:HG23	2.07	0.75
2:B:647:ASN:HD22	2:B:649:LEU:H	1.35	0.75
14:B:1215:CLA:HMB1	14:B:1215:CLA:HBB1	1.68	0.75
14:A:1126:CLA:H93	17:J:4012:BCR:H361	1.69	0.74
14:B:1222:CLA:HAA2	14:B:1223:CLA:OBD	1.87	0.74
1:A:453:PHE:O	14:A:1132:CLA:HBB2	1.88	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:639:ASN:HD22	2:B:642:ASN:HD22	1.36	0.74
2:B:229:TRP:HB2	14:B:1213:CLA:H12	1.70	0.73
2:B:497:ASN:O	2:B:498:VAL:HB	1.87	0.73
4:D:50:ARG:N	4:D:54:ASN:HD21	1.84	0.73
2:B:159:LYS:H	2:B:159:LYS:CD	1.92	0.73
2:B:494:ASN:HD22	2:B:496:GLY:N	1.84	0.72
2:B:181:LEU:HG	14:B:1210:CLA:H43	1.71	0.72
2:B:425:LEU:HG	14:B:1236:CLA:CBB	2.20	0.72
2:B:622:LEU:HD12	14:B:1012:CLA:C1	2.15	0.72
11:M:31:LYS:O	11:M:31:LYS:CG	2.34	0.72
2:B:725:LEU:HD11	14:B:1226:CLA:H203	1.69	0.72
2:B:329:TYR:OH	2:B:340:HIS:HE1	1.71	0.72
3:C:39:ALA:O	20:C:3012:HOH:O	2.07	0.72
2:B:343:CYS:HB3	14:B:1221:CLA:H42	1.72	0.71
14:B:1216:CLA:HAA2	14:B:1221:CLA:HBB1	1.72	0.71
2:B:36:MET:HE3	2:B:40:ASN:HB2	1.72	0.71
1:A:202:ALA:HB2	1:A:312:GLY:HA3	1.71	0.71
1:A:221:LEU:HB2	1:A:222:PRO:HD3	1.73	0.71
1:A:341:HIS:HE1	18:A:5003:LHG:HC11	1.56	0.70
5:E:68:VAL:HG23	5:E:69:ALA:H	1.56	0.70
2:B:222:ALA:HB3	2:B:223:PRO:HD3	1.74	0.69
1:A:255:LYS:HB2	1:A:277:ASP:OD2	1.92	0.69
2:B:589:MET:HE1	2:B:590:LEU:HA	1.75	0.69
1:A:13:ARG:HE	1:A:15:VAL:CG2	2.05	0.68
14:A:1136:CLA:H101	14:L:1502:CLA:H191	1.75	0.68
2:B:602:TRP:HE1	2:B:614:GLN:HE21	1.40	0.68
1:A:221:LEU:HD11	1:A:295:SER:HA	1.76	0.68
1:A:399:TRP:CD1	14:A:1126:CLA:HAB	2.29	0.68
6:F:52:VAL:HG12	6:F:54:ASP:HB2	1.76	0.67
1:A:117:VAL:HG13	1:A:123:GLN:NE2	2.08	0.67
2:B:25:ALA:HA	14:B:1226:CLA:H42	1.76	0.67
1:A:101:GLU:OE2	1:A:155:GLU:HG2	1.95	0.66
6:F:102:ASP:OD2	6:F:105:LEU:HB2	1.95	0.66
9:K:73:VAL:HA	14:K:1401:CLA:HBB1	1.77	0.66
2:B:339:TRP:HZ2	14:B:1221:CLA:HAB	1.58	0.66
1:A:336:PHE:HB2	18:A:5003:LHG:HC41	1.78	0.66
3:C:65:ARG:HG2	3:C:67:TYR:CZ	2.31	0.66
15:A:2001:PQN:H172	17:B:4014:BCR:H382	1.77	0.66
4:D:50:ARG:H	4:D:54:ASN:ND2	1.89	0.66
2:B:188:ALA:HA	14:B:1212:CLA:CBB	2.27	0.65
1:A:352:TRP:HB3	14:A:1103:CLA:HAC1	1.77	0.65
2:B:318:PHE:HB2	14:B:1220:CLA:HMA1	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:210:ASN:O	2:B:214:THR:HG23	1.96	0.65
2:B:318:PHE:CD1	14:B:1219:CLA:HAB	2.32	0.65
2:B:41:LEU:O	2:B:45:ILE:HG12	1.97	0.65
6:F:63:PHE:C	6:F:66:PRO:HD2	2.17	0.65
1:A:249:MET:O	1:A:252:LEU:O	2.15	0.65
1:A:257:ASP:OD1	1:A:262:SER:HB3	1.96	0.65
2:B:492:TRP:CE3	2:B:493:PRO:HD3	2.32	0.65
1:A:269:THR:O	1:A:270:PHE:HB2	1.96	0.65
2:B:313:LYS:O	2:B:314:VAL:HG13	1.97	0.65
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.78	0.65
10:L:6:LYS:HB2	10:L:7:PRO:HD2	1.79	0.65
14:A:1237:CLA:H191	14:L:1502:CLA:HBB1	1.78	0.65
6:F:54:ASP:OD2	12:X:30:TYR:CE2	2.50	0.64
14:B:1226:CLA:HMB1	14:B:1226:CLA:HBB1	1.78	0.64
2:B:304:MET:HG3	2:B:322:HIS:O	1.97	0.64
2:B:647:ASN:ND2	2:B:649:LEU:H	1.95	0.64
1:A:473:ASP:OD1	10:L:69:ARG:NH2	2.31	0.64
10:L:61:PRO:HB3	14:L:1503:CLA:HBB1	1.78	0.64
8:J:12:PRO:HB2	17:J:4013:BCR:H391	1.78	0.64
2:B:641:TYR:HB2	2:B:646:THR:HG22	1.79	0.64
14:B:1203:CLA:H162	14:B:1225:CLA:HBB2	1.80	0.64
6:F:103:VAL:HB	6:F:104:PRO:HD3	1.79	0.63
3:C:23:ASP:OD2	4:D:95:HIS:HD2	1.81	0.63
14:B:1023:CLA:H111	17:B:4017:BCR:H362	1.79	0.63
6:F:63:PHE:O	6:F:66:PRO:HD2	1.98	0.63
14:A:1011:CLA:HAB	14:B:1021:CLA:NA	2.14	0.63
2:B:318:PHE:HA	14:B:1219:CLA:CAB	2.28	0.63
4:D:117:ARG:HG2	4:D:118:SER:O	1.98	0.63
2:B:622:LEU:CD1	14:B:1012:CLA:H11	2.16	0.63
6:F:60:ALA:O	6:F:65:ILE:HG12	1.98	0.62
2:B:321:PRO:HB2	2:B:409:ASN:HA	1.80	0.62
11:M:29:LEU:O	11:M:30:TYR:HB2	1.99	0.62
2:B:166:TRP:CZ2	14:B:1208:CLA:HMA1	2.33	0.62
1:A:177:TRP:HB2	14:A:1109:CLA:HMC3	1.80	0.62
1:A:651:ARG:HB2	2:B:638:ILE:HG23	1.81	0.62
1:A:104:LEU:HD11	1:A:153:THR:HA	1.81	0.62
1:A:86:TRP:HA	14:A:1105:CLA:HBB2	1.82	0.62
2:B:228:ASN:O	2:B:231:VAL:HG23	2.00	0.62
2:B:136:GLN:HE22	2:B:208:TRP:HE1	1.46	0.62
1:A:602:MET:HG2	14:A:1124:CLA:HBC1	1.80	0.62
2:B:647:ASN:HD21	2:B:649:LEU:HB2	1.64	0.62
2:B:480:LEU:C	2:B:482:SER:H	2.02	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:356:LEU:O	1:A:360:LEU:HB2	2.00	0.62
1:A:353:HIS:CD2	1:A:411:HIS:HD1	2.11	0.61
14:A:1237:CLA:HMA1	2:B:694:ALA:CB	2.29	0.61
2:B:278:ALA:CB	14:B:1214:CLA:HBB1	2.29	0.61
1:A:543:ALA:HB1	14:A:1136:CLA:HMB3	1.83	0.61
14:A:1124:CLA:HAA2	14:A:1125:CLA:OBD	2.00	0.61
1:A:429:VAL:O	1:A:433:VAL:HG13	1.99	0.61
2:B:438:GLY:HA3	14:B:1230:CLA:CBB	2.31	0.61
11:M:24:ARG:HG3	11:M:24:ARG:HH11	1.64	0.61
1:A:42:PRO:HG2	6:F:99:ILE:HD13	1.83	0.61
1:A:90:MET:HE3	14:A:1106:CLA:HED2	1.82	0.61
14:B:1234:CLA:HMB2	14:B:1236:CLA:HED1	1.81	0.61
1:A:726:GLN:HG3	18:A:5001:LHG:O9	2.01	0.61
14:A:1801:CLA:HBD	14:A:1801:CLA:H61	1.83	0.61
1:A:453:PHE:O	14:A:1132:CLA:CBB	2.48	0.61
1:A:601:TRP:HH2	14:A:1022:CLA:HBB1	1.66	0.60
10:L:153:PHE:O	10:L:154:ASN:HB2	1.99	0.60
1:A:518:VAL:HG22	1:A:525:ALA:HB3	1.82	0.60
14:B:1203:CLA:H151	14:B:1203:CLA:H102	1.84	0.60
3:C:30:TRP:O	3:C:36:GLY:HA2	2.00	0.60
1:A:303:ALA:HB2	14:A:1116:CLA:HBB1	1.83	0.60
9:K:32:TYR:O	9:K:34:ILE:N	2.34	0.60
1:A:484:PRO:HB3	14:A:1136:CLA:HED3	1.83	0.60
14:A:1011:CLA:HBB1	14:B:1012:CLA:CED	2.31	0.60
1:A:168:MET:CE	1:A:171:LEU:HD23	2.31	0.60
14:A:1013:CLA:H71	14:A:1140:CLA:HMC3	1.83	0.59
1:A:210:LEU:HD21	17:A:4001:BCR:H342	1.84	0.59
1:A:300:HIS:O	1:A:304:ILE:HG12	2.03	0.59
1:A:19:ASP:HA	1:A:181:HIS:O	2.02	0.59
14:B:1227:CLA:HBC1	17:B:4009:BCR:H23C	1.83	0.59
1:A:231:VAL:O	1:A:232:ALA:CB	2.50	0.59
2:B:181:LEU:HD21	14:B:1210:CLA:H12	1.85	0.59
1:A:259:GLY:O	1:A:261:PHE:N	2.35	0.59
14:A:1138:CLA:H43	14:B:1229:CLA:HAA2	1.84	0.59
2:B:642:ASN:HB2	2:B:643:PRO:HD2	1.84	0.59
2:B:36:MET:CE	2:B:41:LEU:N	2.66	0.59
4:D:40:GLU:H	4:D:71:GLN:NE2	2.01	0.59
1:A:257:ASP:CG	1:A:258:TRP:N	2.56	0.59
7:I:7:ALA:HB1	7:I:10:LEU:HD22	1.83	0.59
2:B:591:ASN:HB2	14:B:1012:CLA:HBC2	1.83	0.58
7:I:37:GLU:C	7:I:38:ALA:OXT	2.41	0.58
2:B:438:GLY:HA3	14:B:1230:CLA:HBB1	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:207:LEU:HD22	17:A:4002:BCR:H361	1.84	0.58
1:A:16:VAL:HG12	1:A:17:ASP:N	2.17	0.58
10:L:36:ALA:HB2	14:L:1502:CLA:HMD1	1.84	0.58
1:A:86:TRP:HA	14:A:1105:CLA:CBB	2.33	0.58
14:B:1230:CLA:O1D	8:J:35:ASP:HA	2.02	0.58
14:A:1121:CLA:HMA1	14:A:1801:CLA:HAC2	1.85	0.58
2:B:589:MET:O	2:B:589:MET:HE2	2.02	0.58
2:B:243:PHE:N	2:B:263:GLN:HE22	1.90	0.58
14:A:1106:CLA:HMC2	14:A:1126:CLA:H142	1.84	0.58
1:A:145:GLN:NE2	1:A:145:GLN:H	2.02	0.58
1:A:744:TRP:HB2	14:A:1126:CLA:HBB1	1.86	0.58
2:B:367:ASP:OD1	2:B:370:THR:HG23	2.03	0.58
2:B:648:ASN:N	2:B:648:ASN:HD22	2.02	0.58
17:A:4011:BCR:HC8	17:A:4011:BCR:H321	1.83	0.58
2:B:380:TYR:CD1	14:B:1224:CLA:HBB1	2.39	0.57
1:A:91:TYR:CZ	1:A:147:TRP:CZ3	2.91	0.57
1:A:392:SER:HB3	14:A:1126:CLA:HMA1	1.87	0.57
2:B:414:VAL:HG11	17:B:4009:BCR:H401	1.85	0.57
6:F:82:ARG:O	6:F:86:ILE:HG12	2.04	0.57
14:A:1013:CLA:H12	2:B:430:LEU:HD12	1.85	0.57
1:A:542:HIS:HB3	14:A:1135:CLA:HBB1	1.87	0.57
2:B:557:LYS:HD2	4:D:124:ASN:OD1	2.04	0.57
2:B:279:ILE:HD11	14:B:1214:CLA:CBC	2.35	0.57
5:E:24:ALA:O	5:E:25:SER:HB3	2.05	0.57
14:A:1106:CLA:H112	14:A:1128:CLA:H203	1.87	0.56
1:A:355:GLN:HG3	14:A:1123:CLA:H152	1.87	0.56
1:A:349:THR:HG22	1:A:350:THR:HG23	1.87	0.56
1:A:694:ARG:HD3	2:B:572:GLY:HA3	1.86	0.56
8:J:15:ALA:O	8:J:19:MET:HB2	2.06	0.56
2:B:282:LEU:HD12	14:B:1216:CLA:HMC1	1.87	0.56
6:F:37:ARG:O	6:F:40:GLN:HG2	2.04	0.56
2:B:678:GLN:NE2	2:B:705:ALA:H	2.03	0.56
1:A:189:TRP:CZ2	14:A:1108:CLA:HMA1	2.40	0.56
1:A:67:ASP:O	1:A:71:LYS:HG3	2.05	0.56
2:B:234:GLN:OE1	2:B:234:GLN:HA	2.06	0.56
2:B:339:TRP:CH2	17:B:4009:BCR:H372	2.40	0.56
1:A:233:ALA:O	1:A:235:ASP:N	2.36	0.56
12:X:20:LEU:HD11	12:X:24:PHE:HE1	1.71	0.56
2:B:279:ILE:HG23	2:B:283:PHE:CE2	2.41	0.56
2:B:339:TRP:CZ2	14:B:1221:CLA:HAB	2.39	0.56
2:B:480:LEU:O	2:B:482:SER:N	2.38	0.56
6:F:76:TRP:CE2	6:F:113:GLY:HA3	2.40	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:A:1011:CLA:HAB	14:B:1021:CLA:C1A	2.36	0.56
1:A:66:GLU:OE2	1:A:186:LYS:HG3	2.05	0.56
12:X:9:TYR:O	12:X:10:ALA:HB2	2.05	0.56
1:A:366:LEU:HD11	14:A:1117:CLA:H71	1.87	0.56
1:A:741:ALA:HB2	17:A:4011:BCR:H323	1.88	0.56
1:A:297:THR:O	1:A:300:HIS:HB3	2.06	0.56
14:A:1102:CLA:HMC3	14:A:1104:CLA:HED2	1.86	0.55
14:A:1130:CLA:H12	14:L:1502:CLA:H93	1.86	0.55
4:D:117:ARG:CG	4:D:121:GLN:HB2	2.33	0.55
2:B:588:TRP:HH2	14:B:1012:CLA:CBB	2.19	0.55
2:B:589:MET:HE1	2:B:590:LEU:CA	2.36	0.55
9:K:40:GLY:O	9:K:41:PRO:C	2.44	0.55
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.41	0.55
2:B:398:VAL:CG2	2:B:547:ALA:HB1	2.36	0.55
2:B:425:LEU:HD13	2:B:538:LEU:HA	1.89	0.55
1:A:681:PHE:CD2	17:A:4011:BCR:H363	2.42	0.55
14:B:1225:CLA:H51	17:B:4006:BCR:H392	1.88	0.55
2:B:261:HIS:CD2	2:B:264:THR:H	2.25	0.55
14:B:1224:CLA:HBC3	19:B:5002:LMG:H421	1.88	0.55
2:B:233:ALA:O	2:B:234:GLN:O	2.25	0.55
1:A:372:GLN:HG3	14:A:1124:CLA:CED	2.37	0.55
1:A:681:PHE:CG	17:A:4011:BCR:H363	2.43	0.54
14:B:1238:CLA:H18	17:I:4018:BCR:H362	1.89	0.54
14:A:1237:CLA:HMA1	2:B:694:ALA:HB1	1.88	0.54
14:A:1116:CLA:H41	14:A:1133:CLA:HAA2	1.88	0.54
1:A:244:LEU:O	1:A:246:PRO:HD3	2.06	0.54
2:B:525:VAL:HG13	14:B:1021:CLA:H141	1.89	0.54
17:A:4007:BCR:H333	17:A:4008:BCR:H333	1.89	0.54
2:B:179:ALA:HB2	2:B:287:GLY:HA3	1.89	0.54
1:A:390:GLN:HA	1:A:390:GLN:HE21	1.71	0.54
1:A:403:PHE:HB3	14:A:1104:CLA:H112	1.90	0.54
10:L:35:PRO:HG3	14:L:1502:CLA:HED2	1.88	0.54
2:B:205:HIS:ND1	20:B:5051:HOH:O	2.24	0.54
4:D:43:THR:O	4:D:44:ALA:HB3	2.07	0.54
2:B:413:ARG:HD3	14:B:1227:CLA:OBD	2.07	0.54
14:B:1216:CLA:HMB2	14:B:1221:CLA:HMA3	1.89	0.54
2:B:318:PHE:HA	14:B:1219:CLA:HAB	1.88	0.54
2:B:157:GLN:O	2:B:161:ARG:HG3	2.08	0.54
2:B:592:THR:O	2:B:596:VAL:HG13	2.08	0.54
1:A:308:PHE:HE2	14:A:1119:CLA:HAB	1.72	0.54
2:B:171:GLU:HB3	2:B:290:TYR:HB3	1.90	0.54
12:X:25:LEU:O	12:X:29:TYR:HD1	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:589:MET:C	2:B:589:MET:HE2	2.29	0.54
1:A:42:PRO:HG3	1:A:47:TRP:CE3	2.42	0.54
2:B:614:GLN:O	2:B:618:SER:HB2	2.08	0.54
2:B:103:PHE:CZ	2:B:651:VAL:HG22	2.42	0.54
5:E:6:LYS:HD3	5:E:22:THR:HG22	1.89	0.54
14:A:1022:CLA:OBD	14:B:1021:CLA:HMB3	2.08	0.53
2:B:212:LEU:HD21	17:B:4006:BCR:H341	1.90	0.53
6:F:52:VAL:CG1	6:F:54:ASP:HB2	2.37	0.53
11:M:24:ARG:HH11	11:M:24:ARG:CG	2.20	0.53
1:A:305:ALA:O	1:A:309:ILE:HG12	2.08	0.53
14:A:1125:CLA:HBB1	14:A:1133:CLA:HMA2	1.89	0.53
14:A:1011:CLA:HMB3	14:B:1012:CLA:OBD	2.09	0.53
14:A:1013:CLA:H142	17:A:4011:BCR:H402	1.90	0.53
14:A:1101:CLA:HED1	8:J:12:PRO:HA	1.90	0.53
6:F:88:VAL:HG11	6:F:97:LYS:CB	2.37	0.53
14:B:1226:CLA:H143	19:B:5002:LMG:H231	1.89	0.53
6:F:53:VAL:HG12	6:F:63:PHE:HB2	1.90	0.53
1:A:466:ARG:O	2:B:646:THR:HG21	2.09	0.53
2:B:479:THR:O	2:B:480:LEU:O	2.27	0.53
14:A:1128:CLA:H111	18:A:5001:LHG:H202	1.90	0.53
8:J:19:MET:CE	8:J:19:MET:HA	2.38	0.53
14:A:1124:CLA:H162	17:A:4007:BCR:H272	1.91	0.53
1:A:622:TRP:O	1:A:633:HIS:HD2	1.92	0.53
10:L:16:HIS:CD2	10:L:17:LEU:H	2.27	0.53
1:A:13:ARG:HE	1:A:15:VAL:HG22	1.72	0.53
1:A:168:MET:HE1	1:A:171:LEU:HD23	1.91	0.53
14:A:1013:CLA:O1A	2:B:531:LEU:HD11	2.10	0.52
1:A:59:ASP:OD2	1:A:353:HIS:HE1	1.91	0.52
14:A:1119:CLA:HMB2	14:A:1123:CLA:HMA3	1.92	0.52
1:A:221:LEU:HD11	1:A:295:SER:CA	2.39	0.52
2:B:406:ASN:HD22	2:B:409:ASN:ND2	1.84	0.52
1:A:296:ASP:HB3	14:A:1116:CLA:HMA1	1.90	0.52
1:A:244:LEU:C	1:A:246:PRO:HD3	2.30	0.52
2:B:430:LEU:HB3	14:B:1229:CLA:HED3	1.90	0.52
6:F:40:GLN:OE1	8:J:40:PRO:O	2.26	0.52
1:A:90:MET:CE	14:A:1106:CLA:HED2	2.39	0.52
2:B:78:GLN:OE1	2:B:78:GLN:HA	2.10	0.52
1:A:356:LEU:HG	1:A:360:LEU:HD22	1.91	0.52
2:B:90:ILE:HB	2:B:111:PRO:HB2	1.91	0.52
6:F:79:TRP:CH2	6:F:120:ALA:HA	2.44	0.52
2:B:36:MET:HE2	2:B:41:LEU:N	2.25	0.52
2:B:217:HIS:CG	2:B:218:PRO:HD2	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:744:TRP:CZ2	14:A:1126:CLA:H43	2.44	0.52
14:A:1133:CLA:HMD2	14:A:1134:CLA:HBB1	1.92	0.52
1:A:578:CYS:HB3	1:A:587:CYS:HA	1.91	0.52
8:J:28:GLU:OE1	8:J:28:GLU:HA	2.09	0.52
2:B:634:SER:O	2:B:638:ILE:HB	2.10	0.52
1:A:77:PHE:CE2	14:A:1108:CLA:HBB1	2.45	0.52
1:A:718:GLN:NE2	5:E:42:LYS:HD3	2.25	0.52
2:B:294:PHE:HE1	14:B:1209:CLA:HMA1	1.75	0.52
1:A:83:VAL:HG11	14:A:1103:CLA:H72	1.92	0.51
1:A:16:VAL:HG11	1:A:183:ARG:HB3	1.92	0.51
2:B:279:ILE:HD11	14:B:1214:CLA:HBC2	1.92	0.51
1:A:226:LEU:HD22	1:A:231:VAL:HG21	1.93	0.51
1:A:259:GLY:C	1:A:261:PHE:H	2.14	0.51
2:B:398:VAL:HG23	2:B:547:ALA:HB1	1.93	0.51
10:L:31:ILE:HA	10:L:34:LEU:HD22	1.92	0.51
1:A:542:HIS:HE1	1:A:612:HIS:ND1	2.09	0.51
1:A:71:LYS:NZ	20:A:5034:HOH:O	2.43	0.51
14:A:1125:CLA:HMB3	14:A:1133:CLA:H12	1.93	0.51
1:A:257:ASP:O	1:A:258:TRP:HB2	2.11	0.51
2:B:456:ILE:HG22	2:B:458:ILE:CD1	2.40	0.51
2:B:159:LYS:HD2	2:B:159:LYS:N	2.03	0.51
14:B:1238:CLA:HBB2	15:B:2002:PQN:H141	1.91	0.51
1:A:303:ALA:CB	14:A:1116:CLA:HBB1	2.40	0.51
1:A:453:PHE:C	14:A:1132:CLA:HBB2	2.31	0.51
2:B:453:GLU:HA	6:F:48:LEU:HD22	1.93	0.51
2:B:379:GLN:OE1	2:B:379:GLN:HA	2.11	0.51
1:A:444:LEU:HB2	14:A:1137:CLA:CBB	2.40	0.51
1:A:118:TRP:CB	17:J:4013:BCR:H323	2.41	0.51
4:D:117:ARG:HG2	4:D:118:SER:N	2.26	0.50
14:B:1216:CLA:HMD1	14:B:1218:CLA:HBB1	1.93	0.50
7:I:30:LEU:O	7:I:34:ILE:HG12	2.11	0.50
1:A:16:VAL:CG1	1:A:17:ASP:N	2.74	0.50
3:C:14:THR:HG22	3:C:27:MET:HG3	1.93	0.50
2:B:638:ILE:HD11	2:B:656:PHE:CE2	2.46	0.50
2:B:464:GLN:HG2	2:B:475:TYR:CE2	2.47	0.50
11:M:30:TYR:O	11:M:31:LYS:OXT	2.29	0.50
2:B:588:TRP:HH2	14:B:1012:CLA:HBB1	1.77	0.50
2:B:339:TRP:HE1	14:B:1221:CLA:C3B	2.23	0.50
14:B:1220:CLA:HBB1	14:B:1227:CLA:HMD2	1.94	0.50
4:D:32:THR:HA	4:D:52:GLY:O	2.12	0.50
14:A:1013:CLA:HBB1	14:B:1012:CLA:NB	2.27	0.50
14:B:1221:CLA:H61	14:B:1223:CLA:H42	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:B:1226:CLA:H8	19:B:5002:LMG:H242	1.94	0.50
2:B:431:PHE:CZ	17:J:4015:BCR:HC41	2.46	0.50
5:E:68:VAL:O	5:E:69:ALA:O	2.30	0.49
7:I:9:PHE:CE1	7:I:10:LEU:HD13	2.46	0.49
1:A:691:PHE:HB2	14:A:1013:CLA:HBC2	1.95	0.49
4:D:101:PHE:HB3	4:D:103:GLU:OE2	2.11	0.49
2:B:340:HIS:HD2	14:B:1202:CLA:OBD	1.95	0.49
2:B:459:GLU:OE2	6:F:50:HIS:ND1	2.40	0.49
2:B:548:ARG:HH22	4:D:124:ASN:ND2	2.10	0.49
2:B:548:ARG:HH22	4:D:124:ASN:CG	2.15	0.49
2:B:664:ALA:C	14:B:1023:CLA:HBB1	2.31	0.49
6:F:80:VAL:HG22	6:F:109:CYS:O	2.13	0.49
14:A:1237:CLA:H52	14:B:1238:CLA:H43	1.93	0.49
10:L:105:GLY:O	10:L:106:SER:HB2	2.11	0.49
2:B:114:ILE:O	14:B:1205:CLA:HMD3	2.13	0.49
2:B:425:LEU:HG	14:B:1236:CLA:HBB1	1.94	0.49
14:A:1117:CLA:HMB1	14:A:1117:CLA:HBB1	1.93	0.49
2:B:458:ILE:N	2:B:458:ILE:HD12	2.28	0.49
4:D:30:THR:O	4:D:80:TYR:HA	2.13	0.49
2:B:162:PRO:HB2	2:B:167:PHE:CE1	2.48	0.49
14:B:1021:CLA:H72	14:B:1012:CLA:CED	2.41	0.49
6:F:84:TYR:O	6:F:88:VAL:HG23	2.13	0.49
14:B:1216:CLA:CMB	14:B:1221:CLA:HMA3	2.42	0.49
5:E:7:VAL:O	5:E:20:VAL:HA	2.13	0.49
2:B:261:HIS:CD2	2:B:263:GLN:H	2.31	0.49
1:A:293:TRP:O	1:A:296:ASP:HB2	2.13	0.49
2:B:487:ILE:HG12	14:B:1232:CLA:HMD3	1.94	0.49
1:A:662:ILE:HD12	2:B:627:ARG:HG3	1.95	0.49
10:L:143:LEU:HD12	10:L:143:LEU:HA	1.61	0.49
2:B:390:PHE:CE1	17:B:4010:BCR:H373	2.48	0.48
2:B:294:PHE:O	2:B:296:ILE:HG22	2.13	0.48
14:B:1203:CLA:H143	14:B:1225:CLA:HBB2	1.95	0.48
2:B:182:PHE:CE2	14:B:1210:CLA:H61	2.48	0.48
2:B:446:VAL:HG13	2:B:451:THR:O	2.13	0.48
14:A:1013:CLA:H71	14:A:1140:CLA:CMC	2.42	0.48
1:A:399:TRP:NE1	14:A:1126:CLA:HAB	2.27	0.48
1:A:120:ILE:C	1:A:122:GLY:H	2.16	0.48
2:B:261:HIS:HD2	2:B:263:GLN:H	1.62	0.48
1:A:444:LEU:HB2	14:A:1137:CLA:HBB1	1.96	0.48
14:B:1221:CLA:H61	14:B:1221:CLA:H41	1.68	0.48
1:A:651:ARG:HG3	2:B:638:ILE:CG2	2.43	0.48
8:J:33:TYR:N	8:J:34:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:TRP:HB3	17:J:4013:BCR:H323	1.94	0.48
14:A:1107:CLA:HMA1	8:J:27:ILE:HD13	1.95	0.48
2:B:271:ASP:HB3	14:B:1214:CLA:HMA1	1.96	0.48
14:B:1203:CLA:H91	19:B:5002:LMG:H401	1.96	0.48
6:F:73:ILE:O	6:F:76:TRP:HB3	2.14	0.48
6:F:109:CYS:O	6:F:112:THR:HB	2.12	0.48
1:A:658:ALA:O	1:A:662:ILE:HG12	2.14	0.48
1:A:283:GLY:O	1:A:508:THR:O	2.32	0.48
6:F:88:VAL:HG13	6:F:97:LYS:HD2	1.95	0.48
8:J:31:ARG:CD	17:J:4013:BCR:H312	2.19	0.48
1:A:360:LEU:CD1	14:A:1128:CLA:HBB1	2.44	0.48
1:A:497:ALA:N	1:A:498:PRO:CD	2.76	0.48
1:A:693:GLY:HA3	2:B:574:CYS:HB2	1.95	0.48
2:B:180:GLY:HA3	14:B:1210:CLA:HBB1	1.96	0.48
9:K:74:VAL:C	9:K:76:GLY:H	2.16	0.48
1:A:203:GLY:O	1:A:207:LEU:HB2	2.14	0.47
11:M:24:ARG:NH1	20:M:155:HOH:O	2.46	0.47
1:A:577:PRO:O	1:A:578:CYS:HB3	2.14	0.47
1:A:686:SER:HB3	1:A:734:HIS:HB2	1.95	0.47
6:F:10:ASP:HB3	20:F:4022:HOH:O	2.14	0.47
14:A:1101:CLA:H8	8:J:16:ALA:HA	1.96	0.47
1:A:691:PHE:HB2	14:A:1013:CLA:CBC	2.44	0.47
14:B:1211:CLA:HAB	14:B:1225:CLA:H13	1.96	0.47
2:B:329:TYR:OH	2:B:340:HIS:CE1	2.61	0.47
1:A:168:MET:O	1:A:172:MET:HB2	2.14	0.47
1:A:74:SER:OG	1:A:180:TYR:HB2	2.15	0.47
2:B:647:ASN:HD22	2:B:649:LEU:N	2.08	0.47
4:D:124:ASN:O	4:D:127:GLN:HB2	2.13	0.47
14:B:1205:CLA:HMB2	14:B:1205:CLA:H142	1.96	0.47
1:A:121:VAL:HB	14:B:1230:CLA:HMD1	1.96	0.47
14:A:1112:CLA:HBA2	14:A:1114:CLA:HMB3	1.96	0.47
1:A:399:TRP:HB3	14:A:1126:CLA:HMC3	1.96	0.47
1:A:56:HIS:CG	14:A:1103:CLA:HAB	2.49	0.47
2:B:525:VAL:CG1	14:B:1021:CLA:H141	2.45	0.47
2:B:693:LEU:HD12	14:L:1502:CLA:H11	1.97	0.47
2:B:313:LYS:O	2:B:314:VAL:CG2	2.60	0.47
2:B:589:MET:CE	2:B:589:MET:C	2.83	0.47
11:M:24:ARG:CG	11:M:24:ARG:NH1	2.78	0.47
1:A:174:PHE:HD2	14:A:1108:CLA:CBC	2.28	0.47
14:A:1103:CLA:HMC3	14:A:1128:CLA:HMA1	1.97	0.47
8:J:40:PRO:O	8:J:41:LEU:HB2	2.14	0.47
1:A:447:VAL:HG21	14:A:1137:CLA:C2C	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:696:LEU:HD11	10:L:36:ALA:HB1	1.97	0.47
2:B:641:TYR:CB	2:B:646:THR:HG22	2.42	0.47
1:A:379:PRO:HB2	14:A:1117:CLA:HAA2	1.96	0.47
14:A:1140:CLA:H172	8:J:19:MET:HG3	1.98	0.46
6:F:88:VAL:CG1	6:F:97:LYS:HB2	2.41	0.46
3:C:65:ARG:HG2	3:C:67:TYR:OH	2.15	0.46
2:B:198:ILE:HB	2:B:199:PRO:HD3	1.96	0.46
14:B:1207:CLA:H42	10:L:81:SER:HA	1.96	0.46
14:B:1217:CLA:HBB1	17:B:4004:BCR:H14C	1.97	0.46
1:A:638:ASN:O	1:A:642:SER:HB2	2.16	0.46
14:A:1140:CLA:H2	14:A:1140:CLA:O1A	2.15	0.46
1:A:603:TYR:OH	14:A:1011:CLA:HED1	2.15	0.46
14:B:1225:CLA:H3A	14:B:1225:CLA:HBA2	1.64	0.46
2:B:39:GLU:O	2:B:43:GLN:HG3	2.15	0.46
3:C:57:CYS:HA	3:C:58:PRO:HD3	1.71	0.46
14:A:1119:CLA:CMB	14:A:1123:CLA:HMA3	2.46	0.46
4:D:34:PRO:O	4:D:51:GLU:HG3	2.16	0.46
10:L:33:ASN:HB3	14:L:1501:CLA:HAC1	1.97	0.46
2:B:386:MET:HE1	17:B:4010:BCR:H361	1.98	0.46
14:B:1235:CLA:H203	6:F:67:SER:HB3	1.98	0.46
1:A:90:MET:HE1	14:A:1106:CLA:HAA2	1.98	0.46
14:B:1012:CLA:H61	14:B:1012:CLA:H41	1.56	0.46
14:A:1118:CLA:HMC1	14:A:1118:CLA:HBC2	1.97	0.46
3:C:61:PHE:HD2	4:D:119:ILE:HG21	1.81	0.46
2:B:361:TYR:O	2:B:364:ILE:HG22	2.15	0.46
1:A:656:ALA:O	1:A:659:SER:HB2	2.16	0.46
11:M:17:LEU:HB3	11:M:18:PRO:CD	2.46	0.46
14:A:1011:CLA:HED1	20:A:5011:HOH:O	2.14	0.46
6:F:80:VAL:HG11	6:F:110:MET:HG2	1.97	0.46
1:A:686:SER:HB3	1:A:734:HIS:CB	2.46	0.46
2:B:479:THR:H	2:B:482:SER:HB3	1.79	0.46
1:A:19:ASP:N	1:A:20:PRO:HD3	2.31	0.46
14:B:1207:CLA:HBB1	14:B:1207:CLA:HHC	1.97	0.46
1:A:744:TRP:CG	17:A:4011:BCR:HC22	2.51	0.46
1:A:445:ASN:ND2	14:B:1023:CLA:HED2	2.31	0.46
3:C:23:ASP:OD2	4:D:95:HIS:CD2	2.67	0.46
17:A:4011:BCR:H381	14:B:1229:CLA:HMA1	1.97	0.46
14:B:1204:CLA:H102	17:I:4018:BCR:HC31	1.98	0.46
1:A:91:TYR:CZ	1:A:147:TRP:HZ3	2.33	0.46
2:B:642:ASN:HB2	2:B:643:PRO:HD3	1.95	0.46
2:B:189:TRP:CA	14:B:1211:CLA:HBB1	2.45	0.46
2:B:738:LYS:O	2:B:739:PHE:CB	2.64	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:M:13:VAL:HG23	17:M:4021:BCR:H402	1.98	0.46
1:A:539:HIS:CG	14:A:1136:CLA:HED2	2.51	0.45
1:A:257:ASP:OD2	1:A:262:SER:C	2.55	0.45
4:D:124:ASN:HB2	4:D:127:GLN:NE2	2.31	0.45
1:A:508:THR:HG21	20:A:5033:HOH:O	2.15	0.45
2:B:468:ALA:O	2:B:482:SER:HB2	2.16	0.45
1:A:44:THR:HB	1:A:720:ARG:HG2	1.98	0.45
1:A:475:PHE:HA	1:A:480:ILE:O	2.16	0.45
14:L:1501:CLA:C1B	14:L:1502:CLA:HED1	2.46	0.45
2:B:509:SER:O	2:B:509:SER:OG	2.25	0.45
14:B:1227:CLA:HBA2	14:B:1227:CLA:H3A	1.49	0.45
2:B:339:TRP:CZ3	17:B:4009:BCR:H372	2.51	0.45
14:B:1225:CLA:H12	17:B:4005:BCR:H393	1.97	0.45
2:B:36:MET:CE	2:B:40:ASN:HB2	2.45	0.45
2:B:589:MET:HE1	2:B:590:LEU:HD23	1.97	0.45
14:B:1217:CLA:H3A	14:B:1217:CLA:HBA2	1.64	0.45
14:A:1120:CLA:H3A	14:A:1120:CLA:HBA2	1.44	0.45
14:A:1123:CLA:HAB	17:A:4007:BCR:H341	1.98	0.45
1:A:91:TYR:CE2	1:A:161:THR:HG21	2.52	0.45
2:B:64:LEU:HD11	17:B:4006:BCR:H271	1.98	0.45
1:A:313:HIS:CE1	17:A:4001:BCR:H363	2.51	0.45
10:L:115:GLU:O	10:L:119:GLN:HG3	2.17	0.45
8:J:22:THR:O	8:J:26:LEU:HD13	2.15	0.45
2:B:471:GLY:HA3	2:B:504:LEU:CD2	2.47	0.45
14:B:1215:CLA:H41	14:B:1215:CLA:H62	1.70	0.45
2:B:220:GLY:HA3	14:B:1212:CLA:HMD1	1.98	0.45
14:A:1118:CLA:H3A	14:A:1118:CLA:HBA2	1.83	0.45
14:B:1213:CLA:H41	14:B:1213:CLA:H62	1.71	0.45
4:D:39:PHE:HB2	4:D:71:GLN:HE21	1.81	0.45
1:A:112:PRO:HB3	1:A:144:PHE:CD1	2.51	0.45
2:B:570:ARG:HH11	2:B:570:ARG:HG3	1.81	0.45
14:B:1229:CLA:HBB1	14:B:1230:CLA:HMB2	1.98	0.45
1:A:508:THR:HG22	1:A:509:ALA:N	2.31	0.45
1:A:168:MET:HE2	1:A:171:LEU:HD23	1.97	0.45
11:M:17:LEU:HB3	11:M:18:PRO:HD3	1.98	0.45
2:B:50:PHE:HB3	2:B:148:ALA:O	2.17	0.45
14:A:1011:CLA:NA	14:B:1021:CLA:HAB	2.31	0.45
2:B:445:VAL:HG21	14:B:1230:CLA:HAC2	1.97	0.45
1:A:321:ILE:HD11	14:A:1118:CLA:H2A	1.99	0.45
1:A:90:MET:HE2	14:A:1126:CLA:HED1	1.99	0.45
1:A:711:LEU:HD23	6:F:130:THR:HG22	1.98	0.45
1:A:445:ASN:ND2	2:B:680:LEU:HD21	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:134:LYS:HG2	4:D:136:TYR:CZ	2.52	0.45
8:J:1:MET:O	8:J:1:MET:HE2	2.17	0.45
1:A:737:LEU:HD22	14:A:1140:CLA:HMA1	1.99	0.45
1:A:86:TRP:HE1	14:A:1106:CLA:HBA1	1.82	0.45
2:B:497:ASN:O	2:B:499:TRP:CE3	2.70	0.45
1:A:250:ALA:HA	1:A:258:TRP:CD1	2.52	0.45
2:B:557:LYS:NZ	4:D:124:ASN:OD1	2.43	0.45
4:D:114:SER:N	20:D:144:HOH:O	2.50	0.45
1:A:75:ALA:HB1	14:A:1103:CLA:HBB1	1.99	0.44
14:A:1104:CLA:H3A	14:A:1128:CLA:HAB	1.99	0.44
14:B:1224:CLA:H3A	14:B:1224:CLA:CGA	2.47	0.44
2:B:215:MET:HA	2:B:216:PRO:HD3	1.83	0.44
2:B:531:LEU:HD21	14:B:1012:CLA:HBB1	1.99	0.44
14:B:1207:CLA:H43	14:B:1207:CLA:CED	2.47	0.44
1:A:92:PHE:CZ	1:A:96:LYS:HG3	2.53	0.44
14:B:1211:CLA:HBA1	17:B:4006:BCR:H383	2.00	0.44
2:B:370:THR:HG21	20:B:5026:HOH:O	2.16	0.44
2:B:480:LEU:C	2:B:482:SER:N	2.70	0.44
5:E:6:LYS:CD	5:E:22:THR:HG22	2.47	0.44
1:A:212:TRP:N	14:A:1112:CLA:HBB1	2.32	0.44
3:C:6:ILE:HD12	3:C:6:ILE:N	2.33	0.44
14:B:1228:CLA:HBC3	17:F:4016:BCR:H362	1.99	0.44
2:B:441:VAL:O	2:B:445:VAL:HG23	2.17	0.44
2:B:48:SER:HB3	14:B:1202:CLA:HBB1	1.98	0.44
14:B:1232:CLA:HMB1	17:B:4010:BCR:HC31	1.98	0.44
14:M:1601:CLA:H3A	14:M:1601:CLA:HBA2	1.69	0.44
2:B:79:ASP:OD2	2:B:82:ASN:HB2	2.18	0.44
1:A:484:PRO:HB3	14:A:1136:CLA:CED	2.47	0.44
4:D:125:PRO:HG3	4:D:135:PRO:HG3	2.00	0.44
1:A:111:LYS:HB2	1:A:130:VAL:HB	2.00	0.44
14:A:1103:CLA:H71	17:A:4003:BCR:H402	2.00	0.44
3:C:65:ARG:HD2	4:D:119:ILE:CD1	2.48	0.44
10:L:56:TYR:OH	14:L:1503:CLA:HED2	2.18	0.44
6:F:132:LYS:HB2	6:F:135:GLU:HG3	1.99	0.44
14:A:1107:CLA:HBC2	14:A:1126:CLA:H141	1.99	0.44
17:A:4011:BCR:H23C	17:A:4011:BCR:H403	1.99	0.44
2:B:430:LEU:HB3	14:B:1229:CLA:CED	2.48	0.44
1:A:642:SER:O	1:A:648:GLY:HA3	2.17	0.44
1:A:462:ASN:HB3	1:A:645:THR:HG22	1.99	0.44
1:A:98:SER:HB2	1:A:113:SER:O	2.18	0.44
2:B:181:LEU:HD13	14:B:1210:CLA:HHB	2.00	0.44
5:E:17:TYR:O	5:E:18:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:A:1140:CLA:H41	14:A:1140:CLA:H62	1.73	0.43
2:B:427:TRP:CE2	14:B:1228:CLA:HBB1	2.53	0.43
14:B:1206:CLA:H102	14:B:1224:CLA:H193	1.99	0.43
2:B:211:PHE:CE2	2:B:212:LEU:HG	2.53	0.43
2:B:236:PRO:O	2:B:250:GLY:HA3	2.18	0.43
1:A:221:LEU:CB	1:A:222:PRO:HD3	2.44	0.43
14:B:1232:CLA:HBA2	14:B:1233:CLA:HMB3	2.00	0.43
2:B:317:PRO:HB3	20:B:5053:HOH:O	2.18	0.43
1:A:519:ALA:HB2	1:A:625:VAL:HG21	2.00	0.43
2:B:529:ILE:HG21	14:B:1234:CLA:HAB	1.99	0.43
10:L:7:PRO:HB3	10:L:12:PRO:HA	2.00	0.43
2:B:439:LEU:HD11	17:J:4015:BCR:H342	2.00	0.43
8:J:1:MET:HE2	8:J:5:LEU:HG	2.01	0.43
2:B:531:LEU:HD21	14:B:1012:CLA:CBB	2.48	0.43
2:B:36:MET:HE1	2:B:41:LEU:N	2.33	0.43
2:B:431:PHE:HD2	14:B:1235:CLA:HBB2	1.84	0.43
2:B:339:TRP:CE2	14:B:1223:CLA:H91	2.54	0.43
14:B:1203:CLA:H41	14:B:1203:CLA:H61	1.60	0.43
2:B:636:GLN:HG3	2:B:737:ALA:CB	2.49	0.43
2:B:305:ASP:OD1	2:B:323:GLN:HA	2.18	0.43
2:B:234:GLN:O	2:B:236:PRO:HD3	2.19	0.43
1:A:91:TYR:CE2	1:A:147:TRP:CZ3	3.07	0.43
14:B:1215:CLA:H3A	14:B:1215:CLA:HBA2	1.92	0.43
14:A:1117:CLA:HMB1	14:A:1117:CLA:CBB	2.48	0.43
1:A:212:TRP:CA	14:A:1112:CLA:HBB1	2.49	0.43
6:F:116:TRP:CG	6:F:117:PRO:HD3	2.54	0.43
1:A:261:PHE:CD2	1:A:261:PHE:O	2.72	0.43
1:A:215:HIS:HB2	14:A:1112:CLA:C1C	2.48	0.43
2:B:231:VAL:C	2:B:234:GLN:HG2	2.36	0.43
14:B:1236:CLA:HBC2	14:X:1701:CLA:HBC3	2.00	0.43
1:A:443:HIS:CD2	14:A:1129:CLA:HMB1	2.53	0.43
6:F:21:ALA:HB2	6:F:35:PHE:CD1	2.54	0.43
17:J:4015:BCR:H20C	17:J:4015:BCR:H361	1.89	0.43
14:B:1205:CLA:O1A	14:B:1224:CLA:HBD	2.19	0.43
1:A:231:VAL:HG11	1:A:236:ILE:HG12	1.99	0.43
5:E:6:LYS:NZ	5:E:22:THR:HG21	2.34	0.43
2:B:24:ILE:HA	14:B:1201:CLA:HMD3	2.01	0.43
4:D:18:LEU:HA	4:D:18:LEU:HD23	1.86	0.43
2:B:325:ILE:HD12	2:B:409:ASN:ND2	2.34	0.42
14:A:1237:CLA:H41	14:A:1237:CLA:H62	1.62	0.42
2:B:36:MET:HE1	2:B:40:ASN:C	2.39	0.42
4:D:73:ARG:HB2	4:D:74:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:A:1402:CLA:H3A	14:A:1402:CLA:HBA2	1.74	0.42
2:B:360:PRO:HG3	14:B:1215:CLA:HBA1	2.00	0.42
1:A:257:ASP:OD1	1:A:262:SER:CB	2.66	0.42
14:A:1117:CLA:O1A	14:A:1127:CLA:HMD1	2.20	0.42
8:J:39:HIS:HA	17:J:4015:BCR:H21C	2.00	0.42
14:B:1207:CLA:CBB	7:I:19:CYS:HB3	2.50	0.42
1:A:514:GLY:HA2	1:A:528:PRO:HB3	2.01	0.42
1:A:683:TRP:CE3	14:A:1011:CLA:HMA1	2.54	0.42
1:A:403:PHE:CB	14:A:1104:CLA:H112	2.49	0.42
1:A:711:LEU:O	1:A:713:VAL:HG22	2.20	0.42
14:B:1229:CLA:H61	17:F:4016:BCR:H312	2.00	0.42
14:B:1214:CLA:HBA2	14:B:1214:CLA:H3A	1.39	0.42
2:B:103:PHE:HZ	2:B:651:VAL:HG22	1.82	0.42
1:A:215:HIS:CD2	1:A:215:HIS:C	2.92	0.42
2:B:357:SER:C	2:B:359:PRO:HD3	2.39	0.42
1:A:360:LEU:HD11	14:A:1128:CLA:HBB1	2.01	0.42
14:A:1107:CLA:H11	17:J:4012:BCR:H19C	2.01	0.42
1:A:234:LYS:HG2	1:A:234:LYS:H	1.68	0.42
2:B:588:TRP:CH2	14:B:1012:CLA:CBB	3.02	0.42
2:B:325:ILE:CD1	2:B:409:ASN:ND2	2.82	0.42
14:A:1124:CLA:H51	14:A:1135:CLA:H43	2.00	0.42
14:B:1226:CLA:HMB1	14:B:1226:CLA:CBB	2.48	0.42
10:L:4:LEU:HD22	10:L:4:LEU:N	2.35	0.42
2:B:535:THR:O	2:B:539:ILE:HG13	2.20	0.42
1:A:679:ALA:HB1	1:A:738:GLY:O	2.20	0.42
2:B:6:LYS:HD2	11:M:31:LYS:HB3	2.02	0.42
2:B:341:LEU:HD21	14:B:1226:CLA:HAB	2.02	0.42
2:B:492:TRP:CZ3	14:B:1233:CLA:HMD3	2.54	0.42
4:D:95:HIS:HA	4:D:97:LYS:N	2.35	0.42
2:B:458:ILE:N	2:B:458:ILE:CD1	2.82	0.42
14:A:1128:CLA:H41	14:A:1128:CLA:H62	1.90	0.42
1:A:120:ILE:O	1:A:122:GLY:N	2.52	0.42
1:A:542:HIS:HD2	20:A:5029:HOH:O	2.03	0.42
1:A:256:VAL:HG12	1:A:257:ASP:N	2.35	0.42
17:A:4011:BCR:H362	14:B:1012:CLA:C4	2.38	0.42
14:A:1126:CLA:H93	17:J:4012:BCR:H20C	2.01	0.42
14:A:1122:CLA:H92	17:A:4007:BCR:H14C	2.01	0.42
2:B:589:MET:HE1	2:B:590:LEU:N	2.35	0.42
1:A:145:GLN:CD	1:A:145:GLN:H	2.22	0.42
2:B:527:HIS:CD2	17:J:4015:BCR:H322	2.55	0.42
18:B:5004:LHG:HC5	12:X:12:ARG:HB3	2.02	0.42
2:B:372:ALA:HA	2:B:600:TRP:CZ3	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:261:HIS:HD2	2:B:264:THR:H	1.67	0.42
1:A:483:GLN:HA	1:A:484:PRO:HD3	1.70	0.42
2:B:414:VAL:HG11	17:B:4009:BCR:C40	2.50	0.42
14:B:1203:CLA:H143	14:B:1225:CLA:CBB	2.50	0.42
6:F:103:VAL:O	6:F:107:ILE:HG13	2.20	0.42
1:A:47:TRP:CZ3	1:A:51:LEU:HD12	2.54	0.42
1:A:511:VAL:HB	1:A:526:MET:HG3	2.02	0.42
1:A:741:ALA:CB	17:A:4011:BCR:H323	2.50	0.42
8:J:19:MET:HE2	8:J:19:MET:HA	2.00	0.42
2:B:136:GLN:HE21	14:B:1211:CLA:HAA1	1.85	0.42
14:A:1108:CLA:HBA2	14:A:1108:CLA:H3A	1.64	0.42
1:A:346:GLU:N	1:A:346:GLU:OE1	2.47	0.42
1:A:336:PHE:CD2	10:L:4:LEU:HD21	2.55	0.41
1:A:42:PRO:CG	6:F:99:ILE:HD13	2.50	0.41
3:C:28:VAL:HG12	4:D:109:ARG:HB3	2.02	0.41
1:A:423:ALA:HA	4:D:38:VAL:HG11	2.02	0.41
1:A:744:TRP:NE1	14:A:1126:CLA:H11	2.35	0.41
1:A:203:GLY:HA3	14:A:1111:CLA:HBB1	2.02	0.41
2:B:189:TRP:HA	14:B:1211:CLA:HBB1	2.02	0.41
7:I:22:MET:O	7:I:26:VAL:HG13	2.19	0.41
3:C:25:LEU:HA	3:C:40:SER:O	2.20	0.41
1:A:686:SER:HB2	1:A:731:GLY:O	2.20	0.41
1:A:156:PHE:CE2	14:A:1114:CLA:HAA2	2.55	0.41
11:M:9:TYR:HB3	17:M:4021:BCR:H401	2.02	0.41
1:A:685:PHE:HA	14:A:1013:CLA:HAB	2.01	0.41
2:B:663:TRP:CE3	14:B:1021:CLA:HMA1	2.56	0.41
4:D:50:ARG:HG3	4:D:50:ARG:NH1	2.35	0.41
14:A:1801:CLA:H12	14:A:1801:CLA:HBA2	1.86	0.41
2:B:178:LEU:O	2:B:283:PHE:HB3	2.21	0.41
1:A:212:TRP:HA	14:A:1112:CLA:HBB1	2.01	0.41
1:A:710:LYS:O	1:A:710:LYS:HD2	2.20	0.41
1:A:49:TRP:CZ3	18:A:5001:LHG:H121	2.56	0.41
14:A:1134:CLA:H3A	14:A:1134:CLA:HBA2	1.73	0.41
1:A:202:ALA:C	14:A:1118:CLA:HBC3	2.41	0.41
6:F:54:ASP:OD2	12:X:30:TYR:HE2	1.98	0.41
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.83	0.41
2:B:691:THR:HA	2:B:692:PRO:HD3	1.90	0.41
1:A:49:TRP:HZ3	18:A:5001:LHG:H121	1.86	0.41
14:B:1213:CLA:HBA2	14:B:1213:CLA:H3A	1.68	0.41
2:B:529:ILE:HG21	14:B:1234:CLA:CAB	2.51	0.41
14:L:1502:CLA:H111	14:L:1502:CLA:H152	1.99	0.41
1:A:161:THR:HG22	17:A:4002:BCR:HC32	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:360:LEU:HA	1:A:360:LEU:HD12	1.93	0.41
14:B:1023:CLA:H122	17:I:4018:BCR:H281	2.03	0.41
4:D:104:LYS:H	4:D:104:LYS:HG2	1.51	0.41
14:A:1119:CLA:HMD1	14:A:1120:CLA:HBB1	2.02	0.41
14:B:1222:CLA:HBA2	14:B:1222:CLA:H3A	1.69	0.41
14:B:1202:CLA:HBA1	14:B:1202:CLA:H3A	1.74	0.41
6:F:73:ILE:O	6:F:77:ILE:HG13	2.21	0.41
1:A:112:PRO:HA	1:A:144:PHE:CE1	2.55	0.41
14:A:1022:CLA:H3A	14:A:1022:CLA:O1A	2.21	0.41
6:F:24:THR:HG21	8:J:35:ASP:OD1	2.20	0.41
14:A:1140:CLA:H52	14:A:1140:CLA:NC	2.36	0.41
14:B:1206:CLA:H203	7:I:26:VAL:CG2	2.51	0.41
2:B:30:PHE:CD1	2:B:45:ILE:HD13	2.56	0.41
1:A:260:PHE:O	1:A:261:PHE:HB2	2.21	0.41
14:A:1117:CLA:H3A	14:A:1117:CLA:HBA2	1.89	0.41
2:B:442:HIS:CD2	2:B:456:ILE:HG13	2.56	0.41
14:B:1207:CLA:H2A	14:B:1207:CLA:O2A	2.20	0.41
10:L:44:ILE:HG23	10:L:45:LEU:N	2.36	0.41
3:C:13:CYS:SG	3:C:15:GLN:HB2	2.61	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.82	0.41
2:B:440:TYR:CZ	2:B:524:LEU:HB3	2.56	0.41
1:A:118:TRP:HB3	17:J:4013:BCR:C32	2.51	0.41
14:A:1013:CLA:C14	17:A:4011:BCR:H402	2.51	0.41
2:B:459:GLU:HA	2:B:460:PRO:HD3	1.81	0.41
14:A:1132:CLA:HED2	10:L:65:LEU:O	2.21	0.41
4:D:43:THR:O	4:D:44:ALA:CB	2.68	0.41
2:B:629:TYR:O	2:B:633:ASN:HB2	2.21	0.41
14:A:1140:CLA:H203	14:F:1301:CLA:CBB	2.52	0.40
14:B:1214:CLA:O1D	14:B:1215:CLA:HMA1	2.21	0.40
14:B:1215:CLA:H3A	14:B:1215:CLA:CGA	2.51	0.40
14:B:1211:CLA:HMA2	17:B:4006:BCR:H282	2.03	0.40
20:A:5047:HOH:O	10:L:16:HIS:HE1	2.04	0.40
6:F:80:VAL:HG21	6:F:110:MET:HA	2.03	0.40
1:A:502:ALA:N	1:A:503:PRO:HD3	2.36	0.40
1:A:713:VAL:HG11	14:A:1138:CLA:HMB3	2.03	0.40
2:B:279:ILE:HD11	14:B:1214:CLA:HBC3	2.02	0.40
5:E:19:GLU:OE1	5:E:42:LYS:NZ	2.52	0.40
2:B:33:HIS:HE1	14:B:1201:CLA:HED1	1.85	0.40
1:A:114:ALA:O	1:A:115:GLN:O	2.39	0.40
2:B:605:LEU:HA	2:B:605:LEU:HD12	1.80	0.40
2:B:53:LEU:HD12	2:B:53:LEU:HA	1.83	0.40
2:B:490:THR:O	2:B:495:TYR:HA	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:A:1126:CLA:H41	14:A:1126:CLA:H62	1.75	0.40
14:A:1130:CLA:HMC2	14:A:1136:CLA:H203	2.03	0.40
14:A:1122:CLA:HHB	14:A:1801:CLA:HBB1	2.02	0.40
2:B:377:HIS:HE2	14:B:1225:CLA:C1B	2.35	0.40
2:B:176:HIS:CG	14:B:1210:CLA:HMC2	2.56	0.40
1:A:212:TRP:O	1:A:216:GLN:HG3	2.22	0.40
10:L:44:ILE:HB	20:L:4045:HOH:O	2.21	0.40
2:B:269:LEU:HD23	2:B:272:MET:HE3	2.02	0.40
2:B:193:LEU:HA	2:B:197:ALA:HB3	2.03	0.40
2:B:564:PRO:O	2:B:565:CYS:HB3	2.22	0.40
17:L:4022:BCR:H361	17:L:4022:BCR:H20C	1.88	0.40
14:A:1116:CLA:CGA	14:A:1116:CLA:H3A	2.52	0.40
2:B:313:LYS:O	2:B:314:VAL:CG1	2.68	0.40
2:B:318:PHE:H	14:B:1219:CLA:C2B	2.34	0.40
3:C:40:SER:HA	20:C:3012:HOH:O	2.21	0.40
4:D:67:LEU:HD12	4:D:71:GLN:HG3	2.03	0.40
2:B:548:ARG:HD3	6:F:141:ARG:O	2.21	0.40
8:J:30:ASN:O	8:J:34:PRO:HG3	2.22	0.40
1:A:120:ILE:HG12	1:A:121:VAL:N	2.36	0.40
1:A:741:ALA:CB	17:A:4011:BCR:C32	2.99	0.40
14:A:1107:CLA:CBB	14:B:1230:CLA:HMD2	2.51	0.40
2:B:496:GLY:O	2:B:497:ASN:C	2.59	0.40
14:B:1220:CLA:CBB	14:B:1227:CLA:HMD2	2.51	0.40
2:B:36:MET:HE3	2:B:40:ASN:CB	2.47	0.40
4:D:88:ASP:HB3	4:D:90:GLU:H	1.86	0.40
20:C:3013:HOH:O	4:D:138:PRO:HG3	2.21	0.40

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:L:4048:HOH:O	20:L:4048:HOH:O[2.655]	1.94	0.26

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%)	695 (94%)	31 (4%)	10 (1%)	16	27
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	19	32
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	18	29
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	10	15
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	2	2
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	10	15
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	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	2	1
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	18	29
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	6	7
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	5	6
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	14	22

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASP
1	A	260	PHE
1	A	261	PHE
2	B	234	GLN
2	B	313	LYS
2	B	314	VAL
2	B	480	LEU
2	B	492	TRP
2	B	497	ASN
2	B	510	GLY
3	C	62	LEU
4	D	2	THR
6	F	91	SER
9	K	41	PRO
9	K	42	GLY
11	M	30	TYR
12	X	10	ALA
1	A	121	VAL
1	A	578	CYS
2	B	565	CYS
4	D	3	LEU

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Mol	Chain	Res	Type
6	F	60	ALA
6	F	89	ARG
10	L	106	SER
1	A	234	LYS
4	D	44	ALA
5	E	53	SER
10	L	104	GLY
1	A	42	PRO
1	A	232	ALA
2	B	481	LEU
5	E	25	SER
5	E	54	GLY
1	A	276	SER
5	E	55	VAL
9	K	56	LEU

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%)	565 (96%)	24 (4%)	41	67
2	B	595/597 (100%)	567 (95%)	28 (5%)	36	61
3	C	67/67 (100%)	66 (98%)	1 (2%)	76	93
4	D	115/115 (100%)	107 (93%)	8 (7%)	21	38
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	107 (98%)	2 (2%)	71	91
7	I	32/32 (100%)	30 (94%)	2 (6%)	25	44
8	J	36/36 (100%)	34 (94%)	2 (6%)	30	51
10	L	117/119 (98%)	109 (93%)	8 (7%)	22	39
11	M	26/26 (100%)	25 (96%)	1 (4%)	44	71
12	X	20/24 (83%)	18 (90%)	2 (10%)	11	20
All	All	1765/1811 (98%)	1687 (96%)	78 (4%)	39	64

All (78) 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	253	TYR
1	A	257	ASP
1	A	260	PHE
1	A	281	PHE
1	A	349	THR
1	A	360	LEU
1	A	372	GLN
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	211	PHE
2	B	214	THR
2	B	256	PHE
2	B	279	ILE
2	B	318	PHE
2	B	349	SER
2	B	370	THR
2	B	411	LEU
2	B	430	LEU
2	B	446	VAL
2	B	479	THR
2	B	525	VAL
2	B	574	CYS
2	B	582	PHE
2	B	589	MET

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Mol	Chain	Res	Type
2	B	596	VAL
2	B	605	LEU
2	B	632	LEU
2	B	635	SER
2	B	647	ASN
2	B	648	ASN
2	B	651	VAL
2	B	697	VAL
2	B	698	ARG
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
4	D	125	PRO
4	D	126	SER
6	F	56	ARG
6	F	105	LEU
7	I	10	LEU
7	I	26	VAL
8	J	1	MET
8	J	19	MET
10	L	4	LEU
10	L	34	LEU
10	L	42	SER
10	L	44	ILE
10	L	48	LEU
10	L	69	ARG
10	L	85	LEU
10	L	134	VAL
11	M	17	LEU
12	X	8	THR
12	X	23	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	50	ASN
1	A	145	GLN

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Mol	Chain	Res	Type
1	A	353	HIS
1	A	359	ASN
1	A	372	GLN
1	A	390	GLN
1	A	426	GLN
1	A	445	ASN
1	A	542	HIS
1	A	633	HIS
1	A	647	ASN
1	A	718	GLN
2	B	33	HIS
2	B	40	ASN
2	B	136	GLN
2	B	261	HIS
2	B	263	GLN
2	B	336	GLN
2	B	340	HIS
2	B	406	ASN
2	B	494	ASN
2	B	611	ASN
2	B	614	GLN
2	B	616	ASN
2	B	639	ASN
2	B	647	ASN
2	B	648	ASN
2	B	678	GLN
2	B	688	HIS
3	C	37	GLN
4	D	54	ASN
4	D	71	GLN
4	D	95	HIS
5	E	18	ASN
6	F	40	GLN
6	F	95	ASN
10	L	16	HIS

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$
14	CLA	A	1011	1	73,73,73	1.62	12 (16%)	95,113,113	2.28	19 (20%)
14	CLA	A	1013	1	73,73,73	1.52	13 (17%)	95,113,113	1.50	19 (20%)
14	CLA	A	1022	20	73,73,73	1.45	11 (15%)	95,113,113	1.51	16 (16%)
14	CLA	A	1101	1	73,73,73	1.46	12 (16%)	95,113,113	1.50	15 (15%)
14	CLA	A	1102	1,14	67,67,73	1.54	11 (16%)	86,105,113	1.59	16 (18%)
14	CLA	A	1103	1	73,73,73	1.33	9 (12%)	95,113,113	1.50	16 (16%)
14	CLA	A	1104	1	73,73,73	1.54	11 (15%)	95,113,113	1.63	20 (21%)
14	CLA	A	1105	1	59,59,73	1.73	11 (18%)	77,96,113	1.57	14 (18%)
14	CLA	A	1106	1	73,73,73	1.50	13 (17%)	95,113,113	1.56	17 (17%)
14	CLA	A	1107	1	73,73,73	1.36	8 (10%)	95,113,113	1.56	18 (18%)
14	CLA	A	1108	1	51,53,73	1.69	11 (21%)	68,89,113	1.56	12 (17%)
14	CLA	A	1109	1,14	73,73,73	1.45	11 (15%)	95,113,113	1.45	16 (16%)
14	CLA	A	1110	1	62,62,73	1.65	13 (20%)	80,99,113	1.60	15 (18%)
14	CLA	A	1111	1	67,68,73	1.49	10 (14%)	87,107,113	1.47	16 (18%)
14	CLA	A	1112	1	51,53,73	1.78	11 (21%)	68,89,113	1.64	15 (22%)
14	CLA	A	1113	1	51,53,73	1.74	11 (21%)	68,89,113	1.59	17 (25%)
14	CLA	A	1114	20	56,57,73	1.70	13 (23%)	73,93,113	1.62	16 (21%)
14	CLA	A	1115	1	62,62,73	1.73	12 (19%)	80,99,113	1.56	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	1116	1	62,62,73	1.70	11 (17%)	80,99,113	1.60	18 (22%)
14	CLA	A	1117	1	73,73,73	1.42	12 (16%)	95,113,113	1.48	18 (18%)
14	CLA	A	1118	1	69,69,73	1.76	15 (21%)	89,108,113	1.60	19 (21%)
14	CLA	A	1119	20	73,73,73	1.37	10 (13%)	95,113,113	1.52	19 (20%)
14	CLA	A	1120	1	56,57,73	1.72	14 (25%)	73,93,113	1.73	17 (23%)
14	CLA	A	1121	1	59,59,73	1.70	11 (18%)	77,96,113	1.60	13 (16%)
14	CLA	A	1122	1	67,67,73	1.48	11 (16%)	86,105,113	1.52	16 (18%)
14	CLA	A	1123	20	73,73,73	1.50	10 (13%)	95,113,113	1.49	16 (16%)
14	CLA	A	1124	20	73,73,73	1.37	10 (13%)	95,113,113	1.39	13 (13%)
14	CLA	A	1125	1	73,73,73	1.55	12 (16%)	95,113,113	1.49	16 (16%)
14	CLA	A	1126	1	73,73,73	1.44	11 (15%)	95,113,113	1.36	15 (15%)
14	CLA	A	1127	1	73,73,73	1.45	12 (16%)	95,113,113	1.40	14 (14%)
14	CLA	A	1128	1	73,73,73	1.64	12 (16%)	95,113,113	1.56	17 (17%)
14	CLA	A	1129	1	58,58,73	1.58	12 (20%)	75,95,113	1.80	18 (24%)
14	CLA	A	1130	1	73,73,73	1.49	9 (12%)	95,113,113	1.44	17 (17%)
14	CLA	A	1131	1	73,73,73	1.35	7 (9%)	95,113,113	1.35	13 (13%)
14	CLA	A	1132	1	73,73,73	1.44	13 (17%)	95,113,113	1.54	15 (15%)
14	CLA	A	1133	1	62,62,73	1.53	13 (20%)	80,99,113	1.63	17 (21%)
14	CLA	A	1134	1	51,53,73	1.69	12 (23%)	68,89,113	1.66	15 (22%)
14	CLA	A	1135	1	59,59,73	1.68	10 (16%)	77,96,113	1.52	18 (23%)
14	CLA	A	1136	1	73,73,73	1.52	10 (13%)	95,113,113	1.40	13 (13%)
14	CLA	A	1137	1	54,55,73	1.83	12 (22%)	72,91,113	1.61	15 (20%)
14	CLA	A	1138	1	73,73,73	1.47	11 (15%)	95,113,113	1.46	15 (15%)
14	CLA	A	1139	20	59,59,73	1.71	10 (16%)	77,96,113	1.55	16 (20%)
14	CLA	A	1140	1	73,73,73	1.50	13 (17%)	95,113,113	1.55	17 (17%)
14	CLA	A	1237	20	73,73,73	1.39	11 (15%)	95,113,113	1.49	16 (16%)
14	CLA	A	1402	-	47,49,73	3.72	14 (29%)	59,83,113	1.76	12 (20%)
14	CLA	A	1801	18	60,60,73	2.01	14 (23%)	79,97,113	1.80	22 (27%)
15	PQN	A	2001	-	34,34,34	3.48	15 (44%)	45,45,45	2.19	3 (6%)
16	SF4	A	3001	1,2	12,12,12	7.82	12 (100%)	0,24,24	0.00	-
17	BCR	A	4001	-	41,41,41	1.32	5 (12%)	56,56,56	1.85	16 (28%)
17	BCR	A	4002	-	41,41,41	1.22	4 (9%)	56,56,56	1.75	16 (28%)
17	BCR	A	4003	-	41,41,41	1.36	7 (17%)	56,56,56	1.92	16 (28%)
17	BCR	A	4007	-	41,41,41	1.31	6 (14%)	56,56,56	1.76	14 (25%)
17	BCR	A	4008	-	41,41,41	1.23	7 (17%)	56,56,56	1.88	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	A	4011	-	41,41,41	1.32	6 (14%)	56,56,56	2.02	20 (35%)
18	LHG	A	5001	-	48,48,48	1.62	6 (12%)	54,54,54	1.22	3 (5%)
18	LHG	A	5003	14	26,26,48	2.27	6 (23%)	31,32,54	1.72	5 (16%)
14	CLA	B	1012	20	73,73,73	1.43	9 (12%)	95,113,113	1.54	17 (17%)
14	CLA	B	1021	2	73,73,73	1.50	12 (16%)	95,113,113	1.46	16 (16%)
14	CLA	B	1023	2	73,73,73	1.59	11 (15%)	95,113,113	1.54	17 (17%)
14	CLA	B	1201	2	62,62,73	1.61	12 (19%)	80,99,113	1.65	16 (20%)
14	CLA	B	1202	2	73,73,73	1.46	9 (12%)	95,113,113	1.41	15 (15%)
14	CLA	B	1203	2	73,73,73	1.47	9 (12%)	95,113,113	1.34	16 (16%)
14	CLA	B	1204	2	73,73,73	1.46	12 (16%)	95,113,113	1.50	14 (14%)
14	CLA	B	1205	2	73,73,73	1.52	10 (13%)	95,113,113	1.54	14 (14%)
14	CLA	B	1206	2	73,73,73	1.30	7 (9%)	95,113,113	1.44	18 (18%)
14	CLA	B	1207	2	73,73,73	1.61	11 (15%)	95,113,113	1.45	18 (18%)
14	CLA	B	1208	2	51,53,73	1.70	11 (21%)	68,89,113	1.64	14 (20%)
14	CLA	B	1209	2	51,53,73	1.75	10 (19%)	68,89,113	1.60	14 (20%)
14	CLA	B	1210	2	73,73,73	1.50	9 (12%)	95,113,113	1.41	16 (16%)
14	CLA	B	1211	2	73,73,73	1.40	12 (16%)	95,113,113	1.52	16 (16%)
14	CLA	B	1212	2	51,53,73	1.75	12 (23%)	68,89,113	1.67	16 (23%)
14	CLA	B	1213	2	62,63,73	1.67	12 (19%)	81,101,113	1.57	14 (17%)
14	CLA	B	1214	2	67,67,73	1.56	11 (16%)	86,105,113	1.64	18 (20%)
14	CLA	B	1215	2	67,68,73	1.54	10 (14%)	87,107,113	1.52	12 (13%)
14	CLA	B	1216	20	73,73,73	1.41	10 (13%)	95,113,113	1.46	14 (14%)
14	CLA	B	1217	2	54,55,73	1.69	10 (18%)	72,91,113	1.71	18 (25%)
14	CLA	B	1218	2	51,53,73	1.75	9 (17%)	68,89,113	1.71	17 (25%)
14	CLA	B	1219	20	62,63,73	1.67	10 (16%)	81,101,113	1.50	14 (17%)
14	CLA	B	1220	2	51,53,73	1.72	9 (17%)	68,89,113	1.59	11 (16%)
14	CLA	B	1221	2	62,62,73	1.78	14 (22%)	80,99,113	1.66	17 (21%)
14	CLA	B	1222	20	53,54,73	1.59	11 (20%)	71,90,113	1.67	20 (28%)
14	CLA	B	1223	2	73,73,73	1.60	13 (17%)	95,113,113	1.40	15 (15%)
14	CLA	B	1224	2	73,73,73	1.53	10 (13%)	95,113,113	1.62	16 (16%)
14	CLA	B	1225	2	73,73,73	1.52	13 (17%)	95,113,113	1.53	17 (17%)
14	CLA	B	1226	2	73,73,73	1.48	14 (19%)	95,113,113	1.44	16 (16%)
14	CLA	B	1227	2	51,53,73	1.64	13 (25%)	68,89,113	1.66	15 (22%)
14	CLA	B	1228	2	56,57,73	1.74	12 (21%)	73,93,113	1.65	13 (17%)
14	CLA	B	1229	2	73,73,73	1.43	9 (12%)	95,113,113	1.53	13 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	1230	2	65,66,73	1.61	13 (20%)	85,104,113	1.56	16 (18%)
14	CLA	B	1231	2	51,53,73	1.80	13 (25%)	68,89,113	1.69	15 (22%)
14	CLA	B	1232	20	51,53,73	1.79	12 (23%)	68,89,113	1.72	15 (22%)
14	CLA	B	1233	20	51,53,73	1.79	11 (21%)	68,89,113	1.60	13 (19%)
14	CLA	B	1234	2	67,68,73	1.59	10 (14%)	87,107,113	1.52	14 (16%)
14	CLA	B	1235	2	73,73,73	1.43	9 (12%)	95,113,113	1.54	17 (17%)
14	CLA	B	1236	2	54,55,73	1.64	12 (22%)	72,91,113	1.63	17 (23%)
14	CLA	B	1238	20	73,73,73	1.44	9 (12%)	95,113,113	1.38	13 (13%)
14	CLA	B	1239	2	73,73,73	1.35	9 (12%)	95,113,113	1.41	15 (15%)
15	PQN	B	2002	-	34,34,34	3.40	14 (41%)	45,45,45	2.05	3 (6%)
17	BCR	B	4004	-	41,41,41	1.48	5 (12%)	56,56,56	1.99	16 (28%)
17	BCR	B	4005	-	41,41,41	1.52	7 (17%)	56,56,56	2.07	19 (33%)
17	BCR	B	4006	-	41,41,41	1.21	5 (12%)	56,56,56	2.00	19 (33%)
17	BCR	B	4009	-	24,25,41	1.61	4 (16%)	31,33,56	1.85	11 (35%)
17	BCR	B	4010	-	41,41,41	1.21	5 (12%)	56,56,56	1.87	17 (30%)
17	BCR	B	4014	-	41,41,41	1.20	4 (9%)	56,56,56	1.98	22 (39%)
17	BCR	B	4017	-	41,41,41	1.24	5 (12%)	56,56,56	1.73	18 (32%)
19	LMG	B	5002	-	55,55,55	0.85	2 (3%)	63,63,63	1.25	3 (4%)
18	LHG	B	5004	-	21,22,48	2.66	5 (23%)	26,28,54	0.98	1 (3%)
16	SF4	C	3002	3	12,12,12	10.15	9 (75%)	0,24,24	0.00	-
16	SF4	C	3003	3	12,12,12	5.90	11 (91%)	0,24,24	0.00	-
14	CLA	F	1301	20	51,53,73	1.81	10 (19%)	68,89,113	1.58	14 (20%)
17	BCR	F	4016	-	41,41,41	1.22	3 (7%)	56,56,56	1.79	14 (25%)
17	BCR	I	4018	-	41,41,41	1.27	6 (14%)	56,56,56	1.77	15 (26%)
17	BCR	I	4020	-	41,41,41	1.24	7 (17%)	56,56,56	1.83	17 (30%)
14	CLA	J	1302	8	51,53,73	1.75	11 (21%)	68,89,113	1.65	17 (25%)
14	CLA	J	1303	8	44,45,73	3.86	11 (25%)	55,78,113	1.86	11 (20%)
17	BCR	J	4012	-	41,41,41	1.23	5 (12%)	56,56,56	1.88	16 (28%)
17	BCR	J	4013	-	41,41,41	1.21	3 (7%)	56,56,56	1.82	20 (35%)
17	BCR	J	4015	-	41,41,41	1.36	6 (14%)	56,56,56	1.85	13 (23%)
14	CLA	K	1401	-	51,53,73	1.86	10 (19%)	68,89,113	1.55	12 (17%)
14	CLA	L	1501	10	73,73,73	1.58	12 (16%)	95,113,113	1.55	14 (14%)
14	CLA	L	1502	10	73,73,73	1.52	12 (16%)	95,113,113	1.47	16 (16%)
14	CLA	L	1503	20	73,73,73	1.46	9 (12%)	95,113,113	1.44	12 (12%)
17	BCR	L	4019	-	41,41,41	1.38	6 (14%)	56,56,56	1.80	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	L	4022	-	41,41,41	1.55	8 (19%)	56,56,56	1.70	12 (21%)
14	CLA	M	1601	20	51,53,73	1.79	11 (21%)	68,89,113	1.65	15 (22%)
17	BCR	M	4021	-	41,41,41	1.29	6 (14%)	56,56,56	1.77	14 (25%)
14	CLA	X	1701	12	51,53,73	1.84	9 (17%)	68,89,113	1.61	15 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1011	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1013	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1022	20	-	0/37/135/135	0/0/9/9
14	CLA	A	1101	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1102	1,14	-	0/29/128/135	0/0/9/9
14	CLA	A	1103	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1104	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1105	1	-	0/21/119/135	0/0/9/9
14	CLA	A	1106	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1107	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1108	1	-	0/11/111/135	0/0/9/9
14	CLA	A	1109	1,14	-	0/37/135/135	0/0/9/9
14	CLA	A	1110	1	-	0/23/122/135	0/0/9/9
14	CLA	A	1111	1	-	0/31/129/135	0/0/9/9
14	CLA	A	1112	1	-	0/11/111/135	0/0/9/9
14	CLA	A	1113	1	-	0/11/111/135	0/0/9/9
14	CLA	A	1114	20	-	0/17/116/135	0/0/9/9
14	CLA	A	1115	1	-	0/23/122/135	0/0/9/9
14	CLA	A	1116	1	-	0/23/122/135	0/0/9/9
14	CLA	A	1117	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1118	1	-	0/33/131/135	0/0/9/9
14	CLA	A	1119	20	-	0/37/135/135	0/0/9/9
14	CLA	A	1120	1	-	0/17/116/135	0/0/9/9
14	CLA	A	1121	1	-	0/21/119/135	0/0/9/9
14	CLA	A	1122	1	-	0/29/128/135	0/0/9/9
14	CLA	A	1123	20	-	0/37/135/135	0/0/9/9
14	CLA	A	1124	20	-	0/37/135/135	0/0/9/9
14	CLA	A	1125	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1126	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1127	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1128	1	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1129	1	-	0/19/117/135	0/0/9/9
14	CLA	A	1130	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1131	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1132	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1133	1	-	0/23/122/135	0/0/9/9
14	CLA	A	1134	1	-	0/11/111/135	0/0/9/9
14	CLA	A	1135	1	-	0/21/119/135	0/0/9/9
14	CLA	A	1136	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1137	1	-	0/16/114/135	0/0/9/9
14	CLA	A	1138	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1139	20	-	0/21/119/135	0/0/9/9
14	CLA	A	1140	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1237	20	-	0/37/135/135	0/0/9/9
14	CLA	A	1402	-	-	0/5/101/135	0/0/9/9
14	CLA	A	1801	18	-	0/22/120/135	0/0/9/9
15	PQN	A	2001	-	-	0/23/43/43	0/0/2/2
16	SF4	A	3001	1,2	-	0/0/48/48	0/0/5/5
17	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
17	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
17	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
17	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
17	BCR	A	4008	-	-	0/29/63/63	0/2/2/2
17	BCR	A	4011	-	-	0/29/63/63	0/2/2/2
18	LHG	A	5001	-	-	0/53/53/53	0/0/0/0
18	LHG	A	5003	14	1/1/5/5	0/31/31/53	0/0/0/0
14	CLA	B	1012	20	-	0/37/135/135	0/0/9/9
14	CLA	B	1021	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1023	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1201	2	-	0/23/122/135	0/0/9/9
14	CLA	B	1202	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1203	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1204	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1205	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1206	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1207	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1208	2	-	0/11/111/135	0/0/9/9
14	CLA	B	1209	2	-	0/11/111/135	0/0/9/9
14	CLA	B	1210	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1211	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1212	2	-	0/11/111/135	0/0/9/9
14	CLA	B	1213	2	-	0/25/123/135	0/0/9/9
14	CLA	B	1214	2	-	0/29/128/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1215	2	-	0/31/129/135	0/0/9/9
14	CLA	B	1216	20	-	0/37/135/135	0/0/9/9
14	CLA	B	1217	2	-	0/16/114/135	0/0/9/9
14	CLA	B	1218	2	-	0/11/111/135	0/0/9/9
14	CLA	B	1219	20	-	0/25/123/135	0/0/9/9
14	CLA	B	1220	2	-	0/11/111/135	0/0/9/9
14	CLA	B	1221	2	-	0/23/122/135	0/0/9/9
14	CLA	B	1222	20	-	0/15/113/135	0/0/9/9
14	CLA	B	1223	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1224	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1225	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1226	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1227	2	-	0/11/111/135	0/0/9/9
14	CLA	B	1228	2	-	0/17/116/135	0/0/9/9
14	CLA	B	1229	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1230	2	-	0/29/127/135	0/0/9/9
14	CLA	B	1231	2	-	0/11/111/135	0/0/9/9
14	CLA	B	1232	20	-	0/11/111/135	0/0/9/9
14	CLA	B	1233	20	-	0/11/111/135	0/0/9/9
14	CLA	B	1234	2	-	0/31/129/135	0/0/9/9
14	CLA	B	1235	2	-	0/37/135/135	0/0/9/9
14	CLA	B	1236	2	-	0/16/114/135	0/0/9/9
14	CLA	B	1238	20	-	0/37/135/135	0/0/9/9
14	CLA	B	1239	2	-	0/37/135/135	0/0/9/9
15	PQN	B	2002	-	-	0/23/43/43	0/0/2/2
17	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
17	BCR	B	4005	-	-	0/29/63/63	0/2/2/2
17	BCR	B	4006	-	-	0/29/63/63	0/2/2/2
17	BCR	B	4009	-	-	0/18/35/63	0/1/1/2
17	BCR	B	4010	-	-	0/29/63/63	0/2/2/2
17	BCR	B	4014	-	-	0/29/63/63	0/2/2/2
17	BCR	B	4017	-	-	0/29/63/63	0/2/2/2
19	LMG	B	5002	-	-	0/50/70/70	0/1/1/1
18	LHG	B	5004	-	-	0/26/26/53	0/0/0/0
16	SF4	C	3002	3	-	0/0/48/48	0/0/5/5
16	SF4	C	3003	3	-	0/0/48/48	0/0/5/5
14	CLA	F	1301	20	-	0/11/111/135	0/0/9/9
17	BCR	F	4016	-	-	0/29/63/63	0/2/2/2
17	BCR	I	4018	-	-	0/29/63/63	0/2/2/2
17	BCR	I	4020	-	-	0/29/63/63	0/2/2/2
14	CLA	J	1302	8	-	0/11/111/135	0/0/9/9
14	CLA	J	1303	8	-	0/2/96/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	J	4012	-	-	0/29/63/63	0/2/2/2
17	BCR	J	4013	-	-	0/29/63/63	0/2/2/2
17	BCR	J	4015	-	-	0/29/63/63	0/2/2/2
14	CLA	K	1401	-	-	0/11/111/135	0/0/9/9
14	CLA	L	1501	10	-	0/37/135/135	0/0/9/9
14	CLA	L	1502	10	-	0/37/135/135	0/0/9/9
14	CLA	L	1503	20	-	0/37/135/135	0/0/9/9
17	BCR	L	4019	-	-	0/29/63/63	0/2/2/2
17	BCR	L	4022	-	-	0/29/63/63	0/2/2/2
14	CLA	M	1601	20	-	0/11/111/135	0/0/9/9
17	BCR	M	4021	-	-	0/29/63/63	0/2/2/2
14	CLA	X	1701	12	-	0/11/111/135	0/0/9/9

All (1264) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	3002	SF4	S1-FE2	-19.48	2.20	2.33
14	A	1402	CLA	CBD-CAD	17.96	1.57	1.41
14	J	1303	CLA	CBD-CAD	17.49	1.57	1.41
16	C	3002	SF4	S4-FE3	-16.81	2.21	2.33
16	C	3002	SF4	S3-FE4	-15.01	2.23	2.33
16	C	3002	SF4	S2-FE1	-13.81	2.24	2.33
14	J	1303	CLA	CBD-CHA	13.24	1.53	1.41
14	A	1402	CLA	CBD-CHA	12.58	1.52	1.41
16	A	3001	SF4	S2-FE3	-11.90	2.25	2.33
16	A	3001	SF4	S4-FE1	-10.83	2.26	2.33
15	A	2001	PQN	C12-C13	9.82	1.52	1.32
15	B	2002	PQN	C12-C13	9.82	1.52	1.32
16	C	3003	SF4	S1-FE4	-9.69	2.26	2.33
16	A	3001	SF4	S1-FE4	-9.58	2.26	2.33
16	A	3001	SF4	S1-FE2	-9.00	2.27	2.33
15	A	2001	PQN	O4-C4	8.90	1.42	1.23
16	C	3003	SF4	S3-FE2	-8.68	2.27	2.33
14	A	1801	CLA	C7-C6	-8.65	1.51	1.55
15	B	2002	PQN	O4-C4	8.59	1.42	1.23
15	A	2001	PQN	O1-C1	8.56	1.42	1.23
16	A	3001	SF4	S3-FE2	-8.10	2.27	2.33
15	B	2002	PQN	O1-C1	8.07	1.41	1.23
18	B	5004	LHG	P-O5	7.89	1.81	1.51
16	A	3001	SF4	S2-FE4	-7.60	2.28	2.33
18	A	5001	LHG	P-O5	7.49	1.79	1.51
16	C	3002	SF4	S2-FE4	-7.05	2.28	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	5003	LHG	P-O5	7.01	1.78	1.51
16	A	3001	SF4	S1-FE3	-6.95	2.28	2.33
15	A	2001	PQN	C2M-C2	-6.79	1.36	1.51
14	B	1207	CLA	C1B-C2B	6.64	1.48	1.40
16	C	3003	SF4	S2-FE4	-6.58	2.28	2.33
16	C	3003	SF4	S4-FE1	-6.53	2.28	2.33
14	A	1135	CLA	C1B-C2B	6.52	1.48	1.40
16	A	3001	SF4	S2-FE1	-6.50	2.28	2.33
14	A	1130	CLA	C1B-C2B	6.47	1.48	1.40
15	B	2002	PQN	C2M-C2	-6.44	1.37	1.51
16	A	3001	SF4	S4-FE2	-6.41	2.28	2.33
16	C	3003	SF4	S1-FE2	-6.40	2.28	2.33
16	C	3002	SF4	S1-FE3	-6.38	2.29	2.33
14	B	1023	CLA	C3B-C4B	6.38	1.50	1.40
16	C	3003	SF4	S2-FE3	-6.27	2.29	2.33
14	A	1118	CLA	C16-C15	-6.12	1.52	1.55
14	J	1303	CLA	C1B-C2B	6.08	1.47	1.40
16	C	3002	SF4	S4-FE2	-6.03	2.29	2.33
14	A	1011	CLA	C1B-C2B	6.01	1.47	1.40
14	F	1301	CLA	C1B-C2B	5.92	1.47	1.40
14	B	1232	CLA	C3B-C4B	5.92	1.49	1.40
14	A	1128	CLA	C3B-C4B	5.89	1.49	1.40
14	B	1231	CLA	C1B-C2B	5.81	1.47	1.40
14	X	1701	CLA	C1B-C2B	5.78	1.47	1.40
14	A	1111	CLA	C1B-C2B	5.77	1.47	1.40
14	B	1203	CLA	C1B-C2B	5.77	1.47	1.40
14	A	1402	CLA	C1B-C2B	5.71	1.47	1.40
14	B	1212	CLA	C3B-C4B	5.69	1.49	1.40
14	A	1115	CLA	C3B-C4B	5.67	1.49	1.40
14	A	1112	CLA	C3B-C4B	5.65	1.49	1.40
14	M	1601	CLA	C1B-C2B	5.62	1.47	1.40
14	B	1223	CLA	C1B-C2B	5.62	1.47	1.40
14	A	1125	CLA	C1B-C2B	5.60	1.47	1.40
14	A	1136	CLA	C3B-C4B	5.60	1.49	1.40
14	A	1022	CLA	C3B-C4B	5.59	1.49	1.40
14	B	1205	CLA	C1B-C2B	5.58	1.47	1.40
14	B	1233	CLA	C1B-C2B	5.57	1.47	1.40
14	B	1221	CLA	C3B-C4B	5.55	1.49	1.40
14	A	1139	CLA	C5-C3	5.54	1.58	1.51
14	A	1137	CLA	C1B-C2B	5.53	1.47	1.40
14	A	1136	CLA	C1B-C2B	5.53	1.47	1.40
14	A	1118	CLA	C3B-C4B	5.52	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1125	CLA	C3B-C4B	5.50	1.49	1.40
14	B	1224	CLA	C3B-C4B	5.47	1.49	1.40
14	B	1235	CLA	C3B-C4B	5.46	1.49	1.40
14	B	1219	CLA	C1B-C2B	5.46	1.47	1.40
14	A	1101	CLA	C3B-C4B	5.43	1.49	1.40
14	B	1218	CLA	C3B-C4B	5.43	1.49	1.40
14	X	1701	CLA	C3B-C4B	5.42	1.49	1.40
14	A	1118	CLA	C1B-C2B	5.42	1.46	1.40
14	L	1502	CLA	C1B-C2B	5.42	1.46	1.40
14	B	1209	CLA	C1B-C2B	5.41	1.46	1.40
14	B	1204	CLA	C3B-C4B	5.37	1.48	1.40
14	B	1202	CLA	C1B-C2B	5.37	1.46	1.40
14	J	1303	CLA	C3B-C4B	5.37	1.48	1.40
14	B	1204	CLA	C1B-C2B	5.36	1.46	1.40
14	A	1104	CLA	C1B-C2B	5.33	1.46	1.40
14	B	1220	CLA	C3B-C4B	5.33	1.48	1.40
14	B	1217	CLA	C1B-C2B	5.32	1.46	1.40
14	A	1119	CLA	C3B-C4B	5.32	1.48	1.40
14	F	1301	CLA	C3B-C4B	5.31	1.48	1.40
14	A	1109	CLA	C1B-C2B	5.30	1.46	1.40
14	B	1213	CLA	C3B-C4B	5.30	1.48	1.40
18	B	5004	LHG	P-O6	5.30	1.83	1.59
14	A	1123	CLA	C3B-C4B	5.30	1.48	1.40
14	A	1138	CLA	C1B-C2B	5.29	1.46	1.40
14	B	1228	CLA	C3B-C4B	5.29	1.48	1.40
14	B	1219	CLA	C3B-C4B	5.28	1.48	1.40
14	A	1013	CLA	C1B-C2B	5.28	1.46	1.40
14	A	1801	CLA	C3B-C4B	5.27	1.48	1.40
14	L	1501	CLA	C3B-C4B	5.27	1.48	1.40
14	B	1238	CLA	C1B-C2B	5.27	1.46	1.40
14	A	1140	CLA	C3B-C4B	5.27	1.48	1.40
14	A	1138	CLA	C3B-C4B	5.26	1.48	1.40
14	B	1229	CLA	C3B-C4B	5.25	1.48	1.40
14	A	1129	CLA	C3B-C4B	5.25	1.48	1.40
14	A	1105	CLA	C1B-C2B	5.24	1.46	1.40
14	M	1601	CLA	C3B-C4B	5.24	1.48	1.40
14	K	1401	CLA	CBA-CGA	-5.23	1.46	1.49
14	B	1231	CLA	C3B-C4B	5.22	1.48	1.40
14	B	1214	CLA	C3B-C4B	5.22	1.48	1.40
14	B	1234	CLA	C3B-C4B	5.21	1.48	1.40
14	A	1110	CLA	C1B-C2B	5.20	1.46	1.40
14	L	1501	CLA	C1B-C2B	5.19	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1134	CLA	C1B-C2B	5.18	1.46	1.40
14	B	1209	CLA	C3B-C4B	5.18	1.48	1.40
14	B	1226	CLA	C1B-C2B	5.17	1.46	1.40
14	B	1233	CLA	C3B-C4B	5.17	1.48	1.40
14	B	1222	CLA	C1B-C2B	5.15	1.46	1.40
14	B	1210	CLA	C1B-C2B	5.14	1.46	1.40
14	A	1113	CLA	C1B-C2B	5.14	1.46	1.40
14	A	1126	CLA	C1B-C2B	5.13	1.46	1.40
14	B	1230	CLA	C1B-C2B	5.13	1.46	1.40
14	B	1239	CLA	C1C-NC	-5.10	1.34	1.38
14	A	1120	CLA	C3B-C4B	5.10	1.48	1.40
14	A	1131	CLA	C1B-C2B	5.09	1.46	1.40
14	A	1116	CLA	C3B-C4B	5.09	1.48	1.40
14	L	1501	CLA	MG-NA	5.09	2.22	2.07
14	B	1218	CLA	C1B-C2B	5.09	1.46	1.40
14	A	1112	CLA	C1B-C2B	5.07	1.46	1.40
14	B	1223	CLA	C3B-C4B	5.07	1.48	1.40
14	B	1023	CLA	C1B-C2B	5.06	1.46	1.40
14	A	1121	CLA	C3B-C4B	5.06	1.48	1.40
14	B	1221	CLA	MG-NA	5.05	2.22	2.07
14	K	1401	CLA	C3B-C4B	5.04	1.48	1.40
14	K	1401	CLA	C1B-C2B	5.02	1.46	1.40
17	B	4009	BCR	C14-C13	5.02	1.40	1.33
14	B	1234	CLA	C1B-C2B	5.02	1.46	1.40
14	A	1110	CLA	C3B-C4B	5.02	1.48	1.40
14	A	1134	CLA	C3B-C4B	5.02	1.48	1.40
14	A	1115	CLA	C1B-C2B	5.01	1.46	1.40
14	A	1123	CLA	MG-NA	5.01	2.22	2.07
14	L	1502	CLA	C3B-C4B	5.01	1.48	1.40
14	B	1215	CLA	C1B-C2B	4.98	1.46	1.40
14	A	1106	CLA	C3B-C4B	4.97	1.48	1.40
14	B	1216	CLA	C3B-C4B	4.96	1.48	1.40
14	A	1128	CLA	C1B-C2B	4.95	1.46	1.40
14	A	1402	CLA	C3B-C4B	4.94	1.48	1.40
14	A	1104	CLA	C3B-C4B	4.93	1.48	1.40
14	J	1302	CLA	C3B-C4B	4.91	1.48	1.40
14	A	1123	CLA	C1B-C2B	4.90	1.46	1.40
14	B	1210	CLA	MG-NA	4.90	2.21	2.07
14	B	1201	CLA	C3B-C4B	4.90	1.48	1.40
14	B	1217	CLA	C3B-C4B	4.90	1.48	1.40
14	B	1021	CLA	C1B-C2B	4.89	1.46	1.40
14	B	1205	CLA	C3B-C4B	4.87	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1208	CLA	C1B-C2B	4.86	1.46	1.40
14	A	1137	CLA	MG-NA	4.86	2.21	2.07
14	A	1139	CLA	C1B-C2B	4.85	1.46	1.40
14	B	1207	CLA	MG-NA	4.84	2.21	2.07
14	A	1140	CLA	C1B-C2B	4.83	1.46	1.40
14	L	1503	CLA	C3B-C4B	4.83	1.48	1.40
14	A	1103	CLA	C1B-C2B	4.83	1.46	1.40
14	B	1213	CLA	C1B-C2B	4.82	1.46	1.40
14	A	1114	CLA	C3B-C4B	4.82	1.47	1.40
14	A	1121	CLA	C1B-C2B	4.81	1.46	1.40
14	A	1109	CLA	C3B-C4B	4.81	1.47	1.40
14	B	1220	CLA	C1B-C2B	4.80	1.46	1.40
14	B	1221	CLA	C1B-C2B	4.80	1.46	1.40
14	A	1127	CLA	C1B-C2B	4.80	1.46	1.40
14	J	1302	CLA	C1B-C2B	4.80	1.46	1.40
14	B	1208	CLA	C3B-C4B	4.79	1.47	1.40
14	A	1101	CLA	C1B-C2B	4.79	1.46	1.40
14	A	1105	CLA	C3B-C4B	4.79	1.47	1.40
14	A	1130	CLA	C3B-C4B	4.78	1.47	1.40
18	B	5004	LHG	P-O3	4.77	1.80	1.59
14	A	1133	CLA	C1B-C2B	4.76	1.46	1.40
14	A	1013	CLA	C3B-C4B	4.76	1.47	1.40
14	A	1116	CLA	C1B-C2B	4.76	1.46	1.40
15	A	2001	PQN	C3-C2	4.75	1.46	1.35
14	B	1225	CLA	MG-NA	4.74	2.21	2.07
14	A	1115	CLA	MG-NA	4.72	2.21	2.07
17	L	4022	BCR	C1-C6	4.72	1.60	1.53
15	B	2002	PQN	C3-C2	4.71	1.46	1.35
14	B	1235	CLA	C1B-C2B	4.71	1.46	1.40
14	B	1228	CLA	C1B-C2B	4.70	1.46	1.40
14	A	1402	CLA	MG-NA	4.70	2.21	2.07
14	A	1121	CLA	MG-NA	4.70	2.21	2.07
14	B	1239	CLA	C1B-C2B	4.70	1.46	1.40
18	A	5001	LHG	P-O3	4.69	1.80	1.59
14	A	1128	CLA	MG-NA	4.69	2.21	2.07
14	B	1227	CLA	C3B-C4B	4.69	1.47	1.40
14	B	1236	CLA	C1B-C2B	4.68	1.46	1.40
14	A	1112	CLA	MG-NA	4.67	2.21	2.07
14	B	1213	CLA	MG-NA	4.67	2.21	2.07
14	B	1238	CLA	MG-NA	4.67	2.21	2.07
14	B	1210	CLA	C3B-C4B	4.66	1.47	1.40
14	B	1230	CLA	C3B-C4B	4.64	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1220	CLA	MG-NA	4.63	2.20	2.07
14	B	1207	CLA	C3B-C4B	4.62	1.47	1.40
14	B	1201	CLA	C1B-C2B	4.62	1.45	1.40
14	J	1303	CLA	MG-NA	4.62	2.20	2.07
14	A	1108	CLA	MG-NA	4.61	2.20	2.07
14	B	1234	CLA	MG-NA	4.61	2.20	2.07
14	B	1232	CLA	MG-NA	4.60	2.20	2.07
14	A	1111	CLA	C3B-C4B	4.60	1.47	1.40
16	C	3003	SF4	S2-FE1	-4.59	2.30	2.33
14	A	1132	CLA	C1B-C2B	4.59	1.45	1.40
17	B	4005	BCR	C1-C6	4.59	1.60	1.53
14	A	1105	CLA	MG-NA	4.59	2.20	2.07
14	A	1126	CLA	C3B-C4B	4.57	1.47	1.40
14	A	1106	CLA	C1B-C2B	4.56	1.45	1.40
14	A	1128	CLA	C4B-NB	4.55	1.40	1.34
14	B	1012	CLA	C3B-C4B	4.53	1.47	1.40
17	L	4019	BCR	C30-C25	4.53	1.60	1.53
14	A	1237	CLA	C3B-C4B	4.52	1.47	1.40
14	A	1114	CLA	C1B-C2B	4.51	1.45	1.40
14	L	1503	CLA	C1B-C2B	4.51	1.45	1.40
14	A	1116	CLA	MG-NA	4.50	2.20	2.07
14	B	1226	CLA	MG-NA	4.50	2.20	2.07
14	A	1137	CLA	C3B-C4B	4.50	1.47	1.40
17	B	4004	BCR	C30-C25	4.49	1.60	1.53
14	A	1135	CLA	MG-NA	4.47	2.20	2.07
14	A	1107	CLA	C3B-C4B	4.47	1.47	1.40
14	A	1127	CLA	MG-NA	4.46	2.20	2.07
14	B	1012	CLA	MG-NA	4.44	2.20	2.07
14	J	1302	CLA	MG-NA	4.44	2.20	2.07
15	B	2002	PQN	C16-C15	-4.44	1.34	1.52
18	A	5003	LHG	P-O6	4.44	1.79	1.59
14	A	1131	CLA	MG-NA	4.44	2.20	2.07
16	A	3001	SF4	S4-FE3	-4.43	2.30	2.33
14	B	1203	CLA	C3B-C4B	4.42	1.47	1.40
14	A	1122	CLA	C1B-C2B	4.42	1.45	1.40
14	X	1701	CLA	MG-NA	4.42	2.20	2.07
14	A	1139	CLA	MG-NA	4.41	2.20	2.07
14	B	1012	CLA	C1B-C2B	4.41	1.45	1.40
14	A	1124	CLA	C3B-C4B	4.40	1.47	1.40
14	B	1224	CLA	C1B-C2B	4.40	1.45	1.40
14	B	1229	CLA	C1B-C2B	4.38	1.45	1.40
14	A	1138	CLA	C4B-NB	4.38	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1102	CLA	C3B-C4B	4.38	1.47	1.40
14	B	1225	CLA	C3B-C4B	4.38	1.47	1.40
14	B	1212	CLA	C1B-C2B	4.38	1.45	1.40
14	A	1133	CLA	C3B-C4B	4.38	1.47	1.40
14	A	1126	CLA	MG-NA	4.38	2.20	2.07
14	B	1206	CLA	MG-NA	4.37	2.20	2.07
17	L	4022	BCR	C30-C25	4.37	1.60	1.53
14	B	1224	CLA	MG-NA	4.37	2.20	2.07
14	B	1021	CLA	C3B-C4B	4.36	1.47	1.40
14	A	1113	CLA	C3B-C4B	4.35	1.47	1.40
14	B	1214	CLA	C1B-C2B	4.35	1.45	1.40
14	A	1120	CLA	C1B-C2B	4.35	1.45	1.40
14	B	1236	CLA	MG-NA	4.35	2.20	2.07
14	B	1223	CLA	MG-NA	4.35	2.20	2.07
14	A	1108	CLA	C3B-C4B	4.34	1.47	1.40
14	B	1206	CLA	C4B-NB	4.33	1.39	1.34
14	B	1205	CLA	MG-NB	4.33	2.14	2.05
14	A	1102	CLA	MG-NA	4.33	2.20	2.07
14	A	1801	CLA	C1B-C2B	4.33	1.45	1.40
14	B	1222	CLA	C3B-C4B	4.33	1.47	1.40
15	A	2001	PQN	C16-C15	-4.32	1.35	1.52
14	B	1218	CLA	MG-NA	4.32	2.20	2.07
14	B	1211	CLA	C3B-C4B	4.32	1.47	1.40
14	B	1227	CLA	C1B-C2B	4.31	1.45	1.40
14	A	1104	CLA	MG-NA	4.31	2.20	2.07
14	A	1108	CLA	C1B-C2B	4.30	1.45	1.40
14	A	1117	CLA	MG-NA	4.30	2.20	2.07
14	L	1503	CLA	MG-NA	4.30	2.20	2.07
14	A	1127	CLA	C4B-NB	4.29	1.39	1.34
14	B	1202	CLA	MG-NA	4.28	2.19	2.07
14	B	1203	CLA	MG-NA	4.28	2.19	2.07
14	K	1401	CLA	MG-NA	4.28	2.19	2.07
14	B	1228	CLA	C4-C3	4.28	1.55	1.47
14	A	1113	CLA	MG-NA	4.28	2.19	2.07
14	B	1233	CLA	MG-NA	4.27	2.19	2.07
14	B	1212	CLA	MG-NA	4.27	2.19	2.07
14	A	1102	CLA	C1B-C2B	4.27	1.45	1.40
14	B	1216	CLA	MG-NA	4.27	2.19	2.07
14	A	1114	CLA	MG-NA	4.27	2.19	2.07
14	B	1217	CLA	MG-NA	4.27	2.19	2.07
14	B	1207	CLA	C1C-NC	-4.26	1.35	1.38
14	A	1120	CLA	C4-C3	4.26	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	4007	BCR	C30-C25	4.26	1.59	1.53
14	A	1124	CLA	C1B-C2B	4.25	1.45	1.40
14	A	1136	CLA	MG-NA	4.25	2.19	2.07
16	C	3003	SF4	S4-FE2	-4.24	2.30	2.33
14	B	1208	CLA	MG-NA	4.23	2.19	2.07
14	B	1236	CLA	C3B-C4B	4.22	1.47	1.40
14	B	1232	CLA	C1B-C2B	4.21	1.45	1.40
14	A	1011	CLA	C4B-NB	4.20	1.39	1.34
14	B	1224	CLA	C4B-NB	4.20	1.39	1.34
14	A	1101	CLA	MG-NA	4.20	2.19	2.07
14	A	1801	CLA	MG-NA	4.19	2.19	2.07
14	A	1129	CLA	C1B-C2B	4.18	1.45	1.40
14	A	1120	CLA	MG-NA	4.18	2.19	2.07
14	B	1209	CLA	MG-NA	4.17	2.19	2.07
14	F	1301	CLA	MG-NA	4.16	2.19	2.07
14	A	1114	CLA	C4-C3	4.14	1.54	1.47
14	A	1013	CLA	MG-NB	4.13	2.14	2.05
14	L	1501	CLA	C4B-NB	4.12	1.39	1.34
14	A	1134	CLA	MG-NA	4.11	2.19	2.07
14	B	1221	CLA	C4B-NB	4.11	1.39	1.34
14	M	1601	CLA	MG-NA	4.11	2.19	2.07
14	B	1225	CLA	C1B-C2B	4.09	1.45	1.40
14	B	1227	CLA	MG-NA	4.09	2.19	2.07
14	B	1206	CLA	C1B-C2B	4.09	1.45	1.40
14	B	1211	CLA	MG-NA	4.09	2.19	2.07
14	A	1118	CLA	MG-NA	4.09	2.19	2.07
14	F	1301	CLA	C4B-NB	4.07	1.39	1.34
14	B	1215	CLA	MG-NA	4.07	2.19	2.07
14	B	1216	CLA	C1B-C2B	4.07	1.45	1.40
14	A	1011	CLA	MG-NA	4.05	2.19	2.07
14	A	1117	CLA	C3B-C4B	4.04	1.46	1.40
14	A	1237	CLA	C1B-C2B	4.04	1.45	1.40
14	B	1238	CLA	C1C-NC	-4.03	1.35	1.38
14	B	1219	CLA	MG-NA	4.02	2.19	2.07
14	A	1122	CLA	C3B-C4B	4.02	1.46	1.40
18	A	5003	LHG	P-O3	4.02	1.77	1.59
14	B	1021	CLA	MG-NA	4.00	2.19	2.07
14	A	1125	CLA	MG-NA	4.00	2.19	2.07
14	A	1107	CLA	MG-NA	3.98	2.19	2.07
14	A	1103	CLA	C3B-C4B	3.98	1.46	1.40
14	B	1226	CLA	C3B-C4B	3.96	1.46	1.40
15	B	2002	PQN	C10-C5	3.96	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1109	CLA	MG-NA	3.96	2.18	2.07
14	B	1201	CLA	MG-NA	3.95	2.18	2.07
16	C	3003	SF4	S3-FE4	-3.95	2.30	2.33
14	A	1107	CLA	C1B-C2B	3.95	1.45	1.40
16	C	3003	SF4	S1-FE3	-3.94	2.30	2.33
14	B	1215	CLA	C3B-C4B	3.90	1.46	1.40
14	L	1502	CLA	MG-NA	3.90	2.18	2.07
14	A	1124	CLA	C1C-NC	-3.90	1.35	1.38
14	A	1113	CLA	CBA-CGA	-3.89	1.47	1.49
14	A	1139	CLA	C3B-C4B	3.88	1.46	1.40
14	B	1202	CLA	C3B-C4B	3.87	1.46	1.40
14	B	1230	CLA	MG-NA	3.87	2.18	2.07
14	B	1012	CLA	C4B-NB	3.86	1.39	1.34
14	B	1222	CLA	MG-NA	3.85	2.18	2.07
14	A	1122	CLA	MG-NA	3.85	2.18	2.07
14	B	1023	CLA	C4B-NB	3.83	1.39	1.34
14	A	1011	CLA	C3B-CAB	-3.83	1.45	1.49
14	A	1110	CLA	MG-NA	3.81	2.18	2.07
14	A	1128	CLA	MG-NB	3.81	2.13	2.05
14	X	1701	CLA	C4B-NB	3.79	1.39	1.34
14	B	1225	CLA	C2-C3	3.79	1.40	1.32
14	A	1111	CLA	MG-NA	3.79	2.18	2.07
14	A	1119	CLA	MG-NA	3.78	2.18	2.07
14	A	1126	CLA	C1C-NC	-3.77	1.35	1.38
14	A	1133	CLA	MG-NA	3.76	2.18	2.07
14	A	1022	CLA	MG-NA	3.76	2.18	2.07
14	B	1210	CLA	C4B-NB	3.74	1.39	1.34
14	J	1302	CLA	C1A-NA	3.73	1.40	1.32
16	A	3001	SF4	S3-FE1	-3.72	2.30	2.33
14	B	1230	CLA	C1C-NC	-3.72	1.35	1.38
14	A	1135	CLA	C3B-C4B	3.72	1.46	1.40
14	A	1022	CLA	C1B-C2B	3.72	1.44	1.40
14	A	1125	CLA	C4B-NB	3.71	1.39	1.34
14	A	1022	CLA	C4B-NB	3.71	1.39	1.34
18	A	5001	LHG	P-O6	3.71	1.76	1.59
14	A	1106	CLA	MG-NA	3.71	2.18	2.07
14	B	1229	CLA	MG-NA	3.71	2.18	2.07
14	B	1228	CLA	MG-NA	3.70	2.18	2.07
14	B	1223	CLA	C4B-NB	3.70	1.39	1.34
14	B	1215	CLA	C3B-CAB	3.69	1.52	1.49
14	B	1214	CLA	MG-NA	3.69	2.18	2.07
14	B	1205	CLA	MG-NA	3.67	2.18	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1023	CLA	MG-NA	3.67	2.18	2.07
14	J	1303	CLA	C1A-NA	3.67	1.40	1.32
14	B	1211	CLA	C1B-C2B	3.67	1.44	1.40
14	J	1303	CLA	C4B-NB	3.67	1.39	1.34
14	B	1232	CLA	C4B-NB	3.66	1.39	1.34
14	A	1130	CLA	C1A-NA	3.66	1.40	1.32
18	A	5003	LHG	C13-C12	-3.65	1.53	1.55
14	A	1013	CLA	MG-NA	3.65	2.18	2.07
14	A	1117	CLA	C1B-C2B	3.64	1.44	1.40
16	A	3001	SF4	S3-FE4	-3.63	2.30	2.33
16	C	3002	SF4	S2-FE3	3.63	2.35	2.33
14	B	1229	CLA	C4B-NB	3.62	1.39	1.34
14	M	1601	CLA	C1A-NA	3.61	1.40	1.32
14	B	1021	CLA	C4B-NB	3.60	1.39	1.34
14	L	1502	CLA	MG-NB	3.60	2.13	2.05
14	A	1138	CLA	MG-NA	3.59	2.17	2.07
14	A	1136	CLA	MG-NB	3.58	2.13	2.05
14	B	1204	CLA	C1C-NC	-3.58	1.35	1.38
14	A	1107	CLA	C4B-NB	3.58	1.39	1.34
14	A	1115	CLA	C4B-NB	3.57	1.39	1.34
14	B	1222	CLA	C1A-NA	3.57	1.40	1.32
14	B	1228	CLA	C4B-NB	3.57	1.39	1.34
14	A	1115	CLA	MG-NB	3.57	2.12	2.05
14	A	1131	CLA	C1C-NC	-3.55	1.35	1.38
17	B	4004	BCR	C26-C25	3.55	1.40	1.34
14	A	1104	CLA	C1A-NA	3.55	1.40	1.32
14	B	1231	CLA	C4B-NB	3.55	1.39	1.34
14	A	1137	CLA	O2A-C1	3.55	1.50	1.45
14	A	1011	CLA	C1A-NA	3.54	1.40	1.32
18	A	5003	LHG	O7-C7	3.54	1.45	1.34
14	B	1214	CLA	MG-NB	3.54	2.12	2.05
14	A	1131	CLA	C1A-NA	3.53	1.40	1.32
14	B	1218	CLA	C4B-NB	3.53	1.39	1.34
14	A	1402	CLA	C3D-CAD	-3.53	1.43	1.49
14	B	1203	CLA	MG-NB	3.52	2.12	2.05
14	A	1105	CLA	MG-NB	3.52	2.12	2.05
17	A	4003	BCR	C1-C6	3.52	1.58	1.53
14	A	1103	CLA	MG-NB	3.50	2.12	2.05
14	X	1701	CLA	C1A-NA	3.50	1.40	1.32
14	A	1139	CLA	C1A-NA	3.50	1.40	1.32
14	A	1137	CLA	C1A-NA	3.48	1.39	1.32
17	A	4003	BCR	C30-C25	3.48	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1129	CLA	MG-NA	3.48	2.17	2.07
14	A	1127	CLA	C3B-C4B	3.48	1.45	1.40
14	B	1202	CLA	C1A-NA	3.47	1.39	1.32
14	A	1402	CLA	C1A-NA	3.46	1.39	1.32
14	B	1235	CLA	MG-NA	3.46	2.17	2.07
14	A	1135	CLA	MG-NB	3.46	2.12	2.05
15	A	2001	PQN	C10-C5	3.45	1.46	1.40
14	A	1135	CLA	C1A-NA	3.45	1.39	1.32
17	J	4015	BCR	C30-C25	3.45	1.58	1.53
14	A	1140	CLA	MG-NA	3.44	2.17	2.07
14	A	1132	CLA	C3B-C4B	3.44	1.45	1.40
14	A	1011	CLA	C3B-C4B	3.43	1.45	1.40
14	B	1228	CLA	C1-C2	3.42	1.55	1.49
17	A	4001	BCR	C30-C25	3.42	1.58	1.53
14	B	1205	CLA	C4B-NB	3.41	1.38	1.34
14	B	1223	CLA	C3B-CAB	3.40	1.52	1.49
14	A	1132	CLA	C3B-CAB	-3.40	1.46	1.49
14	B	1233	CLA	C1A-NA	3.40	1.39	1.32
14	A	1801	CLA	C4B-NB	3.39	1.38	1.34
14	A	1132	CLA	MG-NA	3.39	2.17	2.07
14	B	1239	CLA	C3B-C4B	3.39	1.45	1.40
17	J	4013	BCR	C29-C30	3.39	1.62	1.54
14	K	1401	CLA	C4B-NB	3.39	1.38	1.34
14	A	1108	CLA	MG-NB	3.38	2.12	2.05
14	A	1124	CLA	MG-NA	3.38	2.17	2.07
14	A	1105	CLA	C4B-NB	3.37	1.38	1.34
14	B	1210	CLA	MG-NB	3.37	2.12	2.05
14	B	1202	CLA	MG-NB	3.37	2.12	2.05
14	B	1212	CLA	MG-NB	3.36	2.12	2.05
14	B	1204	CLA	C3B-C2B	-3.36	1.35	1.41
14	K	1401	CLA	C1A-NA	3.35	1.39	1.32
14	B	1213	CLA	C1A-NA	3.35	1.39	1.32
17	A	4001	BCR	C1-C6	3.35	1.58	1.53
14	B	1211	CLA	C1A-NA	3.34	1.39	1.32
14	B	1212	CLA	C1A-NA	3.34	1.39	1.32
14	B	1231	CLA	MG-NA	3.34	2.17	2.07
18	B	5004	LHG	O7-C7	3.34	1.44	1.34
14	M	1601	CLA	C4B-NB	3.34	1.38	1.34
14	A	1801	CLA	C1A-NA	3.33	1.39	1.32
14	L	1501	CLA	MG-NB	3.33	2.12	2.05
14	A	1102	CLA	C1A-NA	3.32	1.39	1.32
14	A	1132	CLA	C4B-NB	3.32	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	4011	BCR	C30-C25	3.32	1.58	1.53
14	B	1231	CLA	MG-NB	3.32	2.12	2.05
14	B	1217	CLA	C1A-NA	3.31	1.39	1.32
14	F	1301	CLA	C1A-NA	3.31	1.39	1.32
14	A	1108	CLA	C1A-NA	3.30	1.39	1.32
14	A	1113	CLA	C1A-NA	3.29	1.39	1.32
14	L	1503	CLA	C4B-NB	3.30	1.38	1.34
14	B	1201	CLA	C9-C8	3.29	1.55	1.49
14	A	1130	CLA	MG-NA	3.28	2.16	2.07
14	A	1132	CLA	C3B-C2B	-3.28	1.35	1.41
14	A	1104	CLA	MG-NB	3.27	2.12	2.05
17	A	4002	BCR	C30-C25	3.27	1.58	1.53
14	A	1137	CLA	C4B-NB	3.27	1.38	1.34
16	C	3003	SF4	S3-FE1	-3.27	2.31	2.33
17	J	4013	BCR	C2-C1	3.27	1.62	1.54
14	A	1114	CLA	C1A-NA	3.27	1.39	1.32
14	B	1220	CLA	C1A-NA	3.26	1.39	1.32
14	B	1227	CLA	C3B-C2B	-3.24	1.35	1.41
14	A	1140	CLA	C1C-NC	-3.24	1.35	1.38
14	B	1226	CLA	C1A-NA	3.23	1.39	1.32
14	A	1109	CLA	C1A-NA	3.23	1.39	1.32
14	B	1208	CLA	MG-NB	3.23	2.12	2.05
14	A	1112	CLA	C4B-NB	3.23	1.38	1.34
14	A	1103	CLA	MG-NA	3.22	2.16	2.07
14	B	1217	CLA	C4B-NB	3.22	1.38	1.34
14	A	1108	CLA	C4B-NB	3.22	1.38	1.34
14	A	1123	CLA	C1A-NA	3.22	1.39	1.32
14	B	1234	CLA	C1A-NA	3.21	1.39	1.32
17	M	4021	BCR	C1-C6	3.21	1.58	1.53
14	A	1110	CLA	C4B-NB	3.21	1.38	1.34
14	J	1302	CLA	C4B-NB	3.21	1.38	1.34
14	A	1119	CLA	C1B-C2B	3.21	1.44	1.40
14	B	1223	CLA	C1A-NA	3.21	1.39	1.32
14	A	1101	CLA	C4B-NB	3.20	1.38	1.34
14	B	1235	CLA	MG-NB	3.20	2.12	2.05
14	B	1236	CLA	MG-NB	3.20	2.12	2.05
14	A	1120	CLA	C1A-NA	3.20	1.39	1.32
14	B	1234	CLA	MG-NB	3.20	2.12	2.05
14	A	1122	CLA	C14-C13	3.19	1.54	1.49
14	A	1127	CLA	C1A-NA	3.19	1.39	1.32
17	F	4016	BCR	C2-C1	3.18	1.62	1.54
14	B	1233	CLA	CBA-CGA	-3.18	1.47	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1135	CLA	C3D-CAD	-3.18	1.40	1.47
14	B	1206	CLA	C1A-NA	3.18	1.39	1.32
14	A	1116	CLA	C1A-NA	3.18	1.39	1.32
14	B	1214	CLA	C4B-NB	3.18	1.38	1.34
14	A	1111	CLA	C4B-NB	3.17	1.38	1.34
14	B	1238	CLA	C1A-NA	3.17	1.39	1.32
14	B	1210	CLA	C1A-NA	3.16	1.39	1.32
14	B	1239	CLA	MG-NA	3.16	2.16	2.07
14	A	1237	CLA	MG-NA	3.16	2.16	2.07
14	B	1219	CLA	MG-NB	3.16	2.12	2.05
14	A	1128	CLA	C1A-NA	3.16	1.39	1.32
14	B	1233	CLA	C4B-NB	3.16	1.38	1.34
14	A	1111	CLA	C1A-NA	3.15	1.39	1.32
14	A	1116	CLA	C9-C8	3.15	1.54	1.49
14	A	1106	CLA	CAA-C2A	3.15	1.59	1.54
14	B	1208	CLA	C1A-NA	3.14	1.39	1.32
17	B	4004	BCR	C1-C6	3.14	1.58	1.53
14	A	1102	CLA	C14-C13	3.14	1.54	1.49
14	B	1232	CLA	C1A-NA	3.14	1.39	1.32
14	B	1225	CLA	C4B-NB	3.14	1.38	1.34
14	A	1129	CLA	C4B-NB	3.13	1.38	1.34
17	B	4005	BCR	C26-C25	3.13	1.39	1.34
14	A	1116	CLA	C4B-NB	3.13	1.38	1.34
17	A	4011	BCR	C1-C6	3.13	1.58	1.53
14	A	1134	CLA	C4B-NB	3.12	1.38	1.34
14	A	1138	CLA	MG-NB	3.12	2.12	2.05
14	A	1112	CLA	C1A-NA	3.12	1.39	1.32
14	A	1115	CLA	C1A-NA	3.12	1.39	1.32
14	A	1105	CLA	C1A-NA	3.12	1.39	1.32
14	A	1118	CLA	C1A-NA	3.11	1.39	1.32
14	L	1503	CLA	MG-NB	3.11	2.11	2.05
17	I	4020	BCR	C30-C25	3.10	1.58	1.53
17	J	4015	BCR	C1-C6	3.09	1.58	1.53
14	A	1134	CLA	C1A-NA	3.09	1.39	1.32
17	A	4008	BCR	C1-C6	3.09	1.58	1.53
14	B	1201	CLA	C4B-NB	3.09	1.38	1.34
14	B	1207	CLA	C1B-NB	3.09	1.38	1.34
14	A	1127	CLA	C1C-NC	-3.09	1.35	1.38
14	B	1218	CLA	C1A-NA	3.09	1.39	1.32
14	A	1105	CLA	C5-C3	3.09	1.55	1.51
14	B	1230	CLA	MG-NB	3.09	2.11	2.05
14	B	1220	CLA	MG-NB	3.09	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1209	CLA	C4B-NB	3.09	1.38	1.34
14	B	1208	CLA	C4B-NB	3.08	1.38	1.34
14	B	1219	CLA	C4B-NB	3.08	1.38	1.34
14	A	1106	CLA	C1C-NC	-3.08	1.35	1.38
14	B	1215	CLA	C1A-NA	3.08	1.39	1.32
14	B	1223	CLA	C1C-NC	-3.07	1.35	1.38
14	A	1116	CLA	CAA-C2A	3.07	1.59	1.54
14	B	1220	CLA	C4B-NB	3.07	1.38	1.34
14	B	1231	CLA	C1A-NA	3.07	1.39	1.32
14	B	1205	CLA	C1A-NA	3.07	1.39	1.32
15	B	2002	PQN	C11-C12	3.06	1.55	1.50
14	A	1402	CLA	C4B-NB	3.06	1.38	1.34
14	X	1701	CLA	MG-NB	3.06	2.11	2.05
14	J	1303	CLA	C3D-CAD	-3.06	1.44	1.49
14	L	1503	CLA	C1B-NB	3.05	1.38	1.34
14	A	1117	CLA	C3B-CAB	3.05	1.52	1.49
14	B	1225	CLA	MG-NB	3.04	2.11	2.05
14	B	1229	CLA	C1A-NA	3.04	1.38	1.32
17	L	4022	BCR	C2-C1	3.04	1.61	1.54
14	B	1235	CLA	C3B-C2B	-3.03	1.36	1.41
14	B	1238	CLA	C3B-C4B	3.03	1.45	1.40
14	B	1226	CLA	C3B-CAB	3.03	1.52	1.49
14	B	1239	CLA	C1A-NA	3.03	1.38	1.32
14	A	1121	CLA	MG-NB	3.03	2.11	2.05
14	A	1121	CLA	C1A-NA	3.02	1.38	1.32
14	B	1219	CLA	CAA-C2A	3.02	1.59	1.54
14	A	1122	CLA	C1C-NC	-3.02	1.35	1.38
14	B	1235	CLA	C4B-NB	3.01	1.38	1.34
17	J	4013	BCR	C30-C25	3.01	1.58	1.53
17	B	4010	BCR	C30-C25	3.00	1.58	1.53
14	A	1122	CLA	C4B-NB	3.00	1.38	1.34
14	A	1113	CLA	MG-NB	2.99	2.11	2.05
16	C	3002	SF4	S3-FE2	2.99	2.35	2.33
14	A	1137	CLA	MG-NB	2.99	2.11	2.05
14	A	1125	CLA	C1A-NA	2.99	1.38	1.32
14	A	1137	CLA	CAA-C2A	2.99	1.59	1.54
14	A	1109	CLA	MG-NB	2.98	2.11	2.05
14	A	1115	CLA	C9-C8	2.98	1.54	1.49
14	A	1140	CLA	C4B-NB	2.98	1.38	1.34
14	A	1117	CLA	C2-C3	2.98	1.38	1.32
14	A	1122	CLA	C1A-NA	2.97	1.38	1.32
14	B	1201	CLA	C1A-NA	2.97	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1209	CLA	C1A-NA	2.97	1.38	1.32
14	A	1139	CLA	MG-NB	2.97	2.11	2.05
14	A	1402	CLA	MG-NB	2.96	2.11	2.05
14	B	1207	CLA	C1A-NA	2.96	1.38	1.32
14	A	1110	CLA	C9-C8	2.96	1.54	1.49
14	B	1209	CLA	MG-NB	2.95	2.11	2.05
14	B	1221	CLA	C1A-NA	2.95	1.38	1.32
14	A	1123	CLA	C4B-NB	2.95	1.38	1.34
14	B	1234	CLA	C3B-C2B	-2.95	1.36	1.41
14	B	1213	CLA	CAA-C2A	2.95	1.59	1.54
14	A	1103	CLA	C4B-NB	2.95	1.38	1.34
14	B	1203	CLA	C1A-NA	2.95	1.38	1.32
14	A	1801	CLA	CAA-C2A	2.95	1.59	1.54
14	B	1021	CLA	C1A-NA	2.94	1.38	1.32
14	F	1301	CLA	MG-NB	2.94	2.11	2.05
14	B	1228	CLA	C3B-C2B	-2.94	1.36	1.41
14	B	1221	CLA	C9-C8	2.93	1.54	1.49
17	F	4016	BCR	C30-C25	2.93	1.58	1.53
14	B	1211	CLA	MG-NB	2.93	2.11	2.05
14	B	1211	CLA	C4B-NB	2.93	1.38	1.34
14	A	1103	CLA	C1A-NA	2.93	1.38	1.32
14	B	1232	CLA	CAA-C2A	2.93	1.59	1.54
14	A	1114	CLA	C4B-NB	2.93	1.38	1.34
14	B	1224	CLA	CAA-C2A	2.92	1.59	1.54
14	B	1235	CLA	CHC-C1C	2.92	1.45	1.35
15	B	2002	PQN	C6-C5	2.92	1.44	1.39
14	A	1106	CLA	C1A-NA	2.92	1.38	1.32
14	A	1110	CLA	C1A-NA	2.92	1.38	1.32
17	B	4004	BCR	C2-C1	2.92	1.61	1.54
14	A	1101	CLA	C1A-NA	2.92	1.38	1.32
14	B	1216	CLA	C4B-NB	2.91	1.38	1.34
14	A	1120	CLA	C4B-NB	2.90	1.38	1.34
14	A	1140	CLA	C1A-NA	2.90	1.38	1.32
14	B	1229	CLA	C3B-C2B	-2.90	1.36	1.41
14	A	1135	CLA	CHB-C4A	2.89	1.43	1.36
14	B	1202	CLA	C4B-NB	2.89	1.38	1.34
14	B	1204	CLA	MG-NA	2.89	2.15	2.07
14	A	1119	CLA	CAA-C2A	2.89	1.59	1.54
14	A	1118	CLA	C4B-NB	2.89	1.38	1.34
14	B	1226	CLA	CAA-C2A	2.88	1.59	1.54
14	B	1219	CLA	C1A-NA	2.88	1.38	1.32
14	A	1133	CLA	C1C-NC	-2.88	1.36	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1011	CLA	C3D-CAD	-2.87	1.41	1.47
14	A	1102	CLA	C4B-NB	2.87	1.38	1.34
14	A	1116	CLA	C3B-C2B	-2.87	1.36	1.41
14	A	1132	CLA	C1C-NC	-2.87	1.36	1.38
14	K	1401	CLA	MG-NB	2.87	2.11	2.05
15	A	2001	PQN	C6-C5	2.87	1.44	1.39
14	B	1221	CLA	MG-NB	2.87	2.11	2.05
14	L	1501	CLA	CHC-C1C	2.86	1.45	1.35
14	B	1230	CLA	C4B-NB	2.86	1.38	1.34
14	A	1022	CLA	MG-NB	2.86	2.11	2.05
14	B	1218	CLA	MG-NB	2.86	2.11	2.05
14	A	1102	CLA	C1C-NC	-2.86	1.36	1.38
14	B	1215	CLA	C4B-NB	2.85	1.38	1.34
14	B	1223	CLA	MG-NB	2.85	2.11	2.05
14	B	1219	CLA	C3B-CAB	2.85	1.51	1.49
14	A	1117	CLA	C4B-NB	2.85	1.38	1.34
14	B	1213	CLA	C4B-NB	2.85	1.38	1.34
14	B	1216	CLA	C1A-NA	2.85	1.38	1.32
14	B	1236	CLA	C1A-NA	2.85	1.38	1.32
17	J	4012	BCR	C29-C30	2.84	1.61	1.54
17	A	4007	BCR	C29-C30	2.84	1.61	1.54
17	B	4005	BCR	C30-C25	2.83	1.57	1.53
14	B	1201	CLA	MG-NB	2.83	2.11	2.05
17	B	4017	BCR	C2-C1	2.83	1.61	1.54
14	A	1127	CLA	C3B-CAB	2.83	1.51	1.49
14	J	1303	CLA	MG-NB	2.83	2.11	2.05
14	B	1212	CLA	C4B-NB	2.83	1.38	1.34
14	A	1129	CLA	C3B-C2B	-2.82	1.36	1.41
14	A	1131	CLA	C3B-C4B	2.82	1.44	1.40
14	B	1236	CLA	C4B-NB	2.82	1.38	1.34
14	A	1237	CLA	C1B-NB	2.82	1.38	1.34
14	B	1207	CLA	MG-NB	2.82	2.11	2.05
14	A	1101	CLA	C1C-NC	-2.82	1.36	1.38
14	A	1116	CLA	MG-NB	2.81	2.11	2.05
14	B	1214	CLA	CAA-C2A	2.82	1.59	1.54
14	A	1106	CLA	MG-NB	2.81	2.11	2.05
14	A	1134	CLA	MG-NB	2.81	2.11	2.05
14	B	1224	CLA	OBD-CAD	2.81	1.26	1.22
17	J	4015	BCR	C2-C1	2.81	1.61	1.54
14	L	1502	CLA	C1B-NB	2.81	1.38	1.34
14	A	1119	CLA	C1A-NA	2.81	1.38	1.32
14	B	1023	CLA	CHC-C1C	2.80	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	4015	BCR	C5-C6	2.80	1.38	1.34
14	B	1204	CLA	C1A-NA	2.79	1.38	1.32
17	A	4002	BCR	C2-C1	2.79	1.61	1.54
17	J	4012	BCR	C1-C6	2.79	1.57	1.53
17	A	4011	BCR	C2-C1	2.79	1.61	1.54
14	A	1106	CLA	C3D-CAD	-2.79	1.41	1.47
14	B	1203	CLA	C1C-NC	-2.78	1.36	1.38
14	A	1124	CLA	MG-NB	2.78	2.11	2.05
14	L	1501	CLA	C1B-NB	2.78	1.38	1.34
14	A	1113	CLA	C4B-NB	2.78	1.38	1.34
14	A	1013	CLA	C3B-CAB	2.78	1.51	1.49
14	B	1206	CLA	C3B-C4B	2.78	1.44	1.40
14	B	1226	CLA	C4B-NB	2.78	1.38	1.34
14	J	1302	CLA	MG-NB	2.76	2.11	2.05
14	B	1218	CLA	CHC-C1C	2.76	1.44	1.35
14	B	1239	CLA	MG-NB	2.76	2.11	2.05
14	B	1215	CLA	CAA-C2A	2.75	1.59	1.54
14	B	1023	CLA	C3B-C2B	-2.75	1.36	1.41
14	A	1123	CLA	C3B-C2B	-2.74	1.36	1.41
14	A	1109	CLA	C4B-NB	2.74	1.38	1.34
14	B	1233	CLA	C1C-NC	-2.74	1.36	1.38
14	A	1237	CLA	C1A-NA	2.73	1.38	1.32
14	A	1136	CLA	C4B-NB	2.73	1.38	1.34
14	A	1121	CLA	C1C-NC	-2.73	1.36	1.38
17	A	4003	BCR	C2-C1	2.73	1.61	1.54
14	L	1501	CLA	C1A-NA	2.73	1.38	1.32
17	B	4014	BCR	C29-C30	2.73	1.61	1.54
14	X	1701	CLA	CBA-CGA	-2.73	1.48	1.49
14	A	1126	CLA	C3B-CAB	2.73	1.51	1.49
14	A	1102	CLA	MG-NB	2.73	2.11	2.05
17	A	4002	BCR	C29-C30	2.73	1.61	1.54
14	A	1112	CLA	MG-NB	2.73	2.11	2.05
17	B	4017	BCR	C30-C25	2.72	1.57	1.53
14	L	1503	CLA	C1A-NA	2.72	1.38	1.32
14	A	1136	CLA	C3B-C2B	-2.71	1.36	1.41
14	B	1023	CLA	MG-NB	2.71	2.11	2.05
14	A	1104	CLA	C4B-NB	2.71	1.38	1.34
14	M	1601	CLA	MG-NB	2.71	2.11	2.05
14	A	1106	CLA	C3B-C2B	-2.71	1.36	1.41
14	B	1217	CLA	MG-NB	2.71	2.11	2.05
14	A	1128	CLA	CHC-C1C	2.71	1.44	1.35
14	B	1223	CLA	CHB-C4A	2.71	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1215	CLA	C4A-NA	-2.71	1.33	1.39
17	M	4021	BCR	C2-C1	2.70	1.61	1.54
17	B	4006	BCR	C1-C6	2.70	1.57	1.53
14	A	1022	CLA	C4A-NA	-2.70	1.33	1.39
14	A	1107	CLA	C1A-NA	2.70	1.38	1.32
18	A	5003	LHG	O8-C23	2.70	1.41	1.33
14	B	1208	CLA	C3B-C2B	-2.70	1.36	1.41
14	A	1013	CLA	C4B-NB	2.70	1.38	1.34
14	B	1209	CLA	CHB-C4A	2.70	1.42	1.36
17	B	4006	BCR	C30-C25	2.70	1.57	1.53
17	J	4012	BCR	C30-C25	2.70	1.57	1.53
14	A	1237	CLA	CAA-C2A	2.69	1.58	1.54
14	A	1138	CLA	CHC-C1C	2.69	1.44	1.35
14	A	1128	CLA	C3B-C2B	-2.69	1.36	1.41
17	M	4021	BCR	C29-C30	2.69	1.61	1.54
14	A	1125	CLA	MG-NB	2.69	2.11	2.05
14	A	1120	CLA	C1-C2	2.69	1.54	1.49
14	B	1224	CLA	CHC-C1C	2.69	1.44	1.35
14	L	1502	CLA	CHC-C1C	2.68	1.44	1.35
14	B	1221	CLA	CHC-C1C	2.68	1.44	1.35
14	A	1801	CLA	MG-NB	2.68	2.11	2.05
14	A	1801	CLA	CHC-C1C	2.68	1.44	1.35
14	A	1121	CLA	C5-C3	2.68	1.54	1.51
17	A	4001	BCR	C26-C25	2.68	1.38	1.34
14	L	1502	CLA	C4B-NB	2.68	1.38	1.34
14	A	1106	CLA	CHC-C1C	2.68	1.44	1.35
14	B	1230	CLA	CHB-C4A	2.68	1.42	1.36
14	A	1117	CLA	MG-NB	2.67	2.11	2.05
14	A	1126	CLA	MG-NB	2.67	2.11	2.05
14	A	1125	CLA	C5-C3	2.67	1.57	1.51
14	B	1214	CLA	C1A-NA	2.67	1.38	1.32
14	A	1011	CLA	C4D-C3D	2.67	1.45	1.41
14	A	1139	CLA	CHB-C4A	2.67	1.42	1.36
14	A	1102	CLA	CAA-C2A	2.67	1.58	1.54
14	B	1222	CLA	C1C-NC	-2.66	1.36	1.38
17	B	4005	BCR	C2-C1	2.66	1.60	1.54
14	J	1303	CLA	CHB-C4A	2.66	1.42	1.36
14	B	1231	CLA	CHC-C1C	2.66	1.44	1.35
17	B	4009	BCR	C29-C30	2.66	1.60	1.54
14	A	1130	CLA	C3B-CAB	2.66	1.51	1.49
14	A	1130	CLA	C1C-NC	-2.66	1.36	1.38
14	A	1125	CLA	CHC-C1C	2.65	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	4017	BCR	C29-C30	2.65	1.60	1.54
17	F	4016	BCR	C29-C30	2.65	1.60	1.54
14	B	1213	CLA	MG-NB	2.65	2.10	2.05
14	A	1114	CLA	C1-C2	2.65	1.54	1.49
14	B	1205	CLA	C3B-C2B	-2.65	1.36	1.41
17	B	4006	BCR	C2-C1	2.64	1.60	1.54
14	X	1701	CLA	CHC-C1C	2.64	1.44	1.35
14	L	1502	CLA	C1A-NA	2.64	1.38	1.32
14	A	1110	CLA	C1C-NC	-2.64	1.36	1.38
17	B	4009	BCR	C30-C25	2.64	1.57	1.53
14	A	1105	CLA	C3B-C2B	-2.64	1.36	1.41
14	A	1133	CLA	C1A-NA	2.63	1.38	1.32
14	A	1112	CLA	CHC-C1C	2.63	1.44	1.35
14	A	1120	CLA	MG-NB	2.63	2.10	2.05
17	L	4022	BCR	C26-C25	2.62	1.38	1.34
17	B	4010	BCR	C2-C1	2.62	1.60	1.54
14	X	1701	CLA	CHB-C4A	2.62	1.42	1.36
17	M	4021	BCR	C30-C25	2.62	1.57	1.53
17	A	4001	BCR	C29-C30	2.62	1.60	1.54
14	B	1220	CLA	CHC-C1C	2.62	1.44	1.35
14	B	1236	CLA	C3B-C2B	-2.61	1.36	1.41
17	J	4015	BCR	C29-C30	2.61	1.60	1.54
14	B	1233	CLA	MG-NB	2.61	2.10	2.05
14	A	1108	CLA	C3B-C2B	-2.61	1.36	1.41
14	B	1212	CLA	CHC-C1C	2.61	1.44	1.35
14	B	1234	CLA	C4B-NB	2.61	1.37	1.34
17	B	4006	BCR	C29-C30	2.60	1.60	1.54
14	B	1232	CLA	MG-NB	2.60	2.10	2.05
14	A	1118	CLA	CHC-C1C	2.60	1.44	1.35
14	B	1231	CLA	C3B-C2B	-2.60	1.36	1.41
19	B	5002	LMG	O8-C28	2.59	1.41	1.33
14	A	1111	CLA	MG-NB	2.59	2.10	2.05
14	A	1013	CLA	CAA-C2A	2.59	1.58	1.54
14	B	1232	CLA	C3B-C2B	-2.59	1.36	1.41
14	A	1120	CLA	C1C-NC	-2.59	1.36	1.38
14	M	1601	CLA	CAA-C2A	2.59	1.58	1.54
17	B	4004	BCR	C29-C30	2.59	1.60	1.54
17	A	4002	BCR	C1-C6	2.59	1.57	1.53
14	B	1232	CLA	CHC-C1C	2.58	1.44	1.35
14	A	1119	CLA	CHC-C1C	2.58	1.44	1.35
14	A	1136	CLA	C1A-NA	2.58	1.37	1.32
14	B	1217	CLA	CAA-C2A	2.58	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1121	CLA	C3B-C2B	-2.58	1.36	1.41
14	B	1012	CLA	C1A-NA	2.58	1.37	1.32
18	A	5001	LHG	O8-C23	2.57	1.41	1.33
17	A	4007	BCR	C1-C6	2.58	1.57	1.53
14	A	1119	CLA	C4B-NB	2.57	1.37	1.34
14	B	1214	CLA	C14-C13	2.57	1.53	1.49
14	B	1229	CLA	C4A-NA	-2.57	1.33	1.39
14	A	1120	CLA	CHC-C1C	2.57	1.44	1.35
14	A	1123	CLA	CHC-C1C	2.57	1.44	1.35
14	B	1222	CLA	C4B-NB	2.57	1.37	1.34
17	I	4020	BCR	C2-C1	2.57	1.60	1.54
14	A	1113	CLA	CHB-C4A	2.57	1.42	1.36
17	A	4011	BCR	C29-C30	2.56	1.60	1.54
14	B	1238	CLA	C3D-CAD	-2.56	1.42	1.47
14	A	1127	CLA	CHB-C4A	2.56	1.42	1.36
14	B	1213	CLA	C5-C3	2.56	1.57	1.51
14	B	1234	CLA	CHC-C1C	2.56	1.44	1.35
14	A	1132	CLA	C4A-NA	-2.56	1.33	1.39
17	A	4008	BCR	C30-C25	2.56	1.57	1.53
14	A	1131	CLA	C3D-CAD	-2.55	1.42	1.47
15	A	2001	PQN	C10-C1	-2.55	1.43	1.48
14	B	1213	CLA	C1C-NC	-2.55	1.36	1.38
14	A	1011	CLA	MG-NB	2.55	2.10	2.05
14	B	1216	CLA	C3B-C2B	-2.55	1.36	1.41
17	A	4011	BCR	C14-C13	2.55	1.39	1.35
14	B	1225	CLA	C3B-C2B	-2.54	1.36	1.41
14	A	1129	CLA	CHC-C1C	2.54	1.44	1.35
14	A	1108	CLA	CAA-C2A	2.54	1.58	1.54
17	J	4012	BCR	C2-C1	2.54	1.60	1.54
14	B	1205	CLA	C1B-CHB	-2.53	1.32	1.39
14	B	1221	CLA	C5-C3	2.53	1.57	1.51
14	B	1233	CLA	CHB-C4A	2.53	1.42	1.36
14	B	1238	CLA	C3B-C2B	-2.53	1.36	1.41
17	A	4011	BCR	C23-C22	-2.53	1.40	1.45
14	B	1224	CLA	MG-NC	2.53	2.14	2.07
14	L	1502	CLA	CAA-C2A	2.53	1.58	1.54
14	B	1217	CLA	CHB-C4A	2.53	1.42	1.36
14	A	1118	CLA	MG-NB	2.52	2.10	2.05
14	L	1503	CLA	CHC-C1C	2.52	1.44	1.35
14	B	1230	CLA	C1A-NA	2.52	1.37	1.32
14	A	1117	CLA	CAA-C2A	2.52	1.58	1.54
14	B	1012	CLA	CHC-C1C	2.52	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	4014	BCR	C5-C6	2.52	1.38	1.34
14	A	1117	CLA	C1C-NC	-2.52	1.36	1.38
14	A	1013	CLA	C1C-NC	-2.52	1.36	1.38
17	L	4019	BCR	C29-C30	2.52	1.60	1.54
14	L	1501	CLA	C1C-NC	-2.52	1.36	1.38
14	B	1021	CLA	MG-NB	2.52	2.10	2.05
14	J	1302	CLA	CHC-C1C	2.52	1.44	1.35
14	A	1121	CLA	CAA-C2A	2.52	1.58	1.54
14	B	1012	CLA	MG-NB	2.51	2.10	2.05
14	B	1225	CLA	CAA-C2A	2.51	1.58	1.54
14	B	1228	CLA	C1B-CHB	-2.50	1.32	1.39
14	J	1302	CLA	CHB-C4A	2.50	1.42	1.36
14	B	1216	CLA	MG-NB	2.50	2.10	2.05
17	B	4010	BCR	C1-C6	2.50	1.57	1.53
14	A	1133	CLA	C9-C8	2.50	1.53	1.49
14	B	1207	CLA	C3B-C2B	-2.50	1.36	1.41
14	F	1301	CLA	CHC-C1C	2.49	1.43	1.35
14	M	1601	CLA	CHB-C4A	2.49	1.42	1.36
14	A	1133	CLA	C4B-NB	2.49	1.37	1.34
14	A	1101	CLA	C3D-CAD	-2.49	1.42	1.47
17	I	4018	BCR	C29-C30	2.48	1.60	1.54
14	B	1227	CLA	C4B-NB	2.48	1.37	1.34
14	A	1102	CLA	CHC-C1C	2.48	1.43	1.35
14	A	1121	CLA	C4B-NB	2.48	1.37	1.34
14	A	1114	CLA	C1C-NC	-2.48	1.36	1.38
19	B	5002	LMG	O7-C8	-2.48	1.40	1.46
14	B	1204	CLA	CAA-C2A	2.47	1.58	1.54
14	A	1137	CLA	CHC-C1C	2.47	1.43	1.35
14	A	1114	CLA	MG-NB	2.47	2.10	2.05
14	A	1124	CLA	C3B-CAB	2.47	1.51	1.49
14	A	1130	CLA	CHB-C4A	2.47	1.42	1.36
14	A	1110	CLA	CAA-C2A	2.47	1.58	1.54
18	A	5001	LHG	O7-C7	2.47	1.41	1.34
14	A	1136	CLA	CHC-C1C	2.47	1.43	1.35
14	B	1215	CLA	MG-NB	2.46	2.10	2.05
14	A	1120	CLA	C3B-C2B	-2.46	1.37	1.41
14	A	1118	CLA	CAA-C2A	2.46	1.58	1.54
14	B	1214	CLA	C3B-C2B	-2.46	1.37	1.41
14	A	1112	CLA	C3B-C2B	-2.46	1.37	1.41
17	A	4001	BCR	C2-C1	2.46	1.60	1.54
14	A	1126	CLA	C1A-NA	2.45	1.37	1.32
14	A	1013	CLA	C1B-CHB	-2.45	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1229	CLA	MG-NB	2.45	2.10	2.05
14	B	1207	CLA	C3D-CAD	-2.45	1.42	1.47
14	A	1137	CLA	C3B-C2B	-2.45	1.37	1.41
14	A	1237	CLA	C3B-C2B	-2.45	1.37	1.41
14	B	1223	CLA	CHC-C1C	2.44	1.43	1.35
14	L	1501	CLA	CAA-C2A	2.44	1.58	1.54
14	B	1012	CLA	C4A-NA	-2.44	1.33	1.39
14	B	1201	CLA	CHC-C1C	2.44	1.43	1.35
14	A	1109	CLA	C1C-NC	-2.44	1.36	1.38
14	A	1127	CLA	MG-NB	2.44	2.10	2.05
14	B	1207	CLA	MG-NC	2.44	2.14	2.07
14	A	1140	CLA	CHC-C1C	2.44	1.43	1.35
14	B	1227	CLA	C1A-NA	2.43	1.37	1.32
17	I	4020	BCR	C29-C30	2.43	1.60	1.54
14	A	1119	CLA	C4A-NA	-2.43	1.33	1.39
14	B	1228	CLA	CHC-C1C	2.43	1.43	1.35
17	J	4012	BCR	C26-C25	2.43	1.38	1.34
17	L	4019	BCR	C26-C25	2.43	1.38	1.34
14	B	1228	CLA	C1A-NA	2.42	1.37	1.32
14	A	1129	CLA	C5-C3	2.42	1.53	1.40
14	B	1208	CLA	C4A-NA	-2.42	1.33	1.39
14	B	1212	CLA	C3B-C2B	-2.42	1.37	1.41
14	B	1230	CLA	CAA-C2A	2.42	1.58	1.54
14	B	1202	CLA	C1C-NC	-2.42	1.36	1.38
17	L	4022	BCR	C29-C30	2.42	1.60	1.54
14	B	1222	CLA	MG-NB	2.41	2.10	2.05
14	A	1129	CLA	C1B-CHB	-2.41	1.33	1.39
14	B	1023	CLA	C4A-NA	-2.41	1.34	1.39
14	A	1129	CLA	C1A-NA	2.41	1.37	1.32
14	B	1221	CLA	C3B-C2B	-2.41	1.37	1.41
17	B	4006	BCR	C5-C6	2.41	1.38	1.34
14	B	1227	CLA	MG-NB	2.41	2.10	2.05
14	A	1117	CLA	C1A-NA	2.41	1.37	1.32
14	A	1119	CLA	C1B-CHB	-2.41	1.33	1.39
14	A	1123	CLA	MG-NB	2.41	2.10	2.05
14	A	1801	CLA	C3B-C2B	-2.41	1.37	1.41
14	A	1140	CLA	C1B-NB	2.41	1.37	1.34
14	M	1601	CLA	CHC-C1C	2.40	1.43	1.35
14	A	1135	CLA	C4B-NB	2.40	1.37	1.34
14	A	1022	CLA	C3B-C2B	-2.40	1.37	1.41
14	A	1116	CLA	CHC-C1C	2.40	1.43	1.35
14	A	1105	CLA	C3D-CAD	-2.40	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1128	CLA	C3B-CAB	2.40	1.51	1.49
15	A	2001	PQN	C11-C12	2.40	1.54	1.50
14	A	1402	CLA	C1C-NC	-2.39	1.36	1.38
14	B	1214	CLA	CHC-C1C	2.39	1.43	1.35
17	I	4020	BCR	C26-C25	2.39	1.38	1.34
14	B	1206	CLA	C1C-NC	-2.39	1.36	1.38
17	A	4003	BCR	C26-C25	2.39	1.38	1.34
14	B	1236	CLA	O2A-C1	2.38	1.49	1.45
14	B	1238	CLA	CAA-C2A	2.38	1.58	1.54
17	A	4007	BCR	C2-C1	2.38	1.60	1.54
14	A	1402	CLA	CHB-C4A	2.38	1.42	1.36
14	B	1023	CLA	C1B-CHB	-2.38	1.33	1.39
17	B	4014	BCR	C2-C1	2.38	1.60	1.54
14	B	1203	CLA	C4B-NB	2.38	1.37	1.34
14	A	1105	CLA	CHC-C1C	2.38	1.43	1.35
14	B	1230	CLA	C5-C3	2.37	1.57	1.51
14	A	1022	CLA	C1A-NA	2.37	1.37	1.32
14	A	1109	CLA	C3B-C2B	-2.37	1.37	1.41
14	B	1208	CLA	CAA-C2A	2.37	1.58	1.54
14	A	1103	CLA	CHC-C1C	2.37	1.43	1.35
14	A	1138	CLA	C3D-CAD	-2.37	1.42	1.47
14	B	1224	CLA	MG-NB	2.37	2.10	2.05
14	B	1220	CLA	CBA-CGA	-2.37	1.48	1.49
15	A	2001	PQN	C15-C13	2.37	1.56	1.51
14	B	1213	CLA	C3B-C2B	-2.37	1.37	1.41
14	A	1134	CLA	CHB-C4A	2.36	1.42	1.36
14	B	1021	CLA	C1B-NB	2.36	1.37	1.34
17	M	4021	BCR	C23-C22	-2.36	1.40	1.45
14	A	1101	CLA	MG-NB	2.36	2.10	2.05
14	B	1226	CLA	CHB-C4A	2.36	1.42	1.36
14	A	1140	CLA	MG-NB	2.36	2.10	2.05
14	B	1223	CLA	C1B-NB	2.36	1.37	1.34
14	A	1110	CLA	C3B-C2B	-2.35	1.37	1.41
14	B	1202	CLA	C3B-CAB	2.35	1.51	1.49
17	L	4019	BCR	C19-C18	-2.35	1.40	1.45
14	A	1101	CLA	C3B-C2B	-2.35	1.37	1.41
14	B	1204	CLA	C1B-CHB	-2.35	1.33	1.39
14	A	1132	CLA	C1A-NA	2.35	1.37	1.32
14	A	1118	CLA	C3B-C2B	-2.34	1.37	1.41
14	A	1140	CLA	C1-C2	2.34	1.57	1.49
14	B	1221	CLA	C4A-NA	-2.34	1.34	1.39
14	B	1219	CLA	CHC-C1C	2.34	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1129	CLA	C4A-NA	-2.34	1.34	1.39
14	B	1217	CLA	CHC-C1C	2.34	1.43	1.35
14	J	1303	CLA	CHC-C1C	2.34	1.43	1.35
14	A	1108	CLA	CBA-CGA	-2.34	1.48	1.49
14	B	1227	CLA	C3B-CAB	-2.34	1.47	1.49
15	B	2002	PQN	C9-C10	2.34	1.43	1.39
14	B	1023	CLA	C1A-NA	2.33	1.37	1.32
14	B	1227	CLA	CHC-C1C	2.33	1.43	1.35
14	A	1134	CLA	CHC-C1C	2.33	1.43	1.35
14	B	1021	CLA	C4A-NA	-2.33	1.34	1.39
14	A	1138	CLA	CAA-C2A	2.33	1.58	1.54
14	B	1223	CLA	C3D-CAD	-2.33	1.42	1.47
14	B	1229	CLA	CHC-C1C	2.33	1.43	1.35
14	A	1124	CLA	CAA-C2A	2.33	1.58	1.54
14	J	1302	CLA	CBA-CGA	-2.33	1.48	1.49
14	B	1234	CLA	CHB-C4A	2.32	1.42	1.36
14	A	1131	CLA	MG-NB	2.32	2.10	2.05
14	A	1115	CLA	CHC-C1C	2.31	1.43	1.35
14	A	1134	CLA	C1C-NC	-2.31	1.36	1.38
14	B	1021	CLA	C1C-NC	-2.31	1.36	1.38
14	B	1209	CLA	CBA-CGA	-2.31	1.48	1.49
14	A	1801	CLA	C3D-CAD	-2.31	1.42	1.47
17	B	4005	BCR	C38-C26	2.31	1.54	1.51
17	L	4022	BCR	C38-C26	2.31	1.54	1.51
14	A	1237	CLA	MG-NB	2.31	2.10	2.05
18	B	5004	LHG	O8-C23	2.31	1.43	1.36
14	A	1124	CLA	C1A-NA	2.31	1.37	1.32
14	A	1138	CLA	C1A-NA	2.31	1.37	1.32
15	B	2002	PQN	C11-C3	2.31	1.55	1.51
14	A	1106	CLA	C4B-NB	2.30	1.37	1.34
14	A	1104	CLA	CHC-C1C	2.30	1.43	1.35
14	A	1124	CLA	C1B-CHB	-2.30	1.33	1.39
17	I	4018	BCR	C26-C25	2.30	1.38	1.34
14	B	1225	CLA	C5-C3	2.30	1.56	1.51
17	A	4008	BCR	C29-C30	2.30	1.60	1.54
14	A	1237	CLA	C4-C3	2.30	1.56	1.50
14	B	1228	CLA	MG-NB	2.30	2.10	2.05
14	K	1401	CLA	C3B-C2B	-2.30	1.37	1.41
17	B	4010	BCR	C5-C6	2.30	1.38	1.34
14	B	1021	CLA	C1B-CHB	-2.29	1.33	1.39
14	A	1118	CLA	C1C-NC	-2.29	1.36	1.38
14	L	1502	CLA	C1B-CHB	-2.29	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1122	CLA	CHC-C1C	2.29	1.43	1.35
14	A	1134	CLA	CAA-C2A	2.28	1.58	1.54
14	B	1209	CLA	CHC-C1C	2.28	1.43	1.35
14	A	1134	CLA	C3D-CAD	-2.28	1.42	1.47
17	I	4018	BCR	C30-C25	2.28	1.57	1.53
14	A	1139	CLA	C3B-C2B	-2.28	1.37	1.41
14	B	1216	CLA	C1C-NC	-2.28	1.36	1.38
14	A	1135	CLA	C3B-CAB	2.28	1.51	1.49
14	B	1207	CLA	CHB-C4A	2.28	1.41	1.36
14	A	1022	CLA	CHC-C1C	2.28	1.43	1.35
14	A	1130	CLA	C4B-NB	2.27	1.37	1.34
14	B	1226	CLA	MG-NC	2.27	2.13	2.07
14	A	1125	CLA	CHB-C4A	2.27	1.41	1.36
14	B	1223	CLA	MG-NC	2.27	2.13	2.07
14	B	1214	CLA	C1B-CHB	-2.27	1.33	1.39
14	B	1208	CLA	C1B-CHB	-2.27	1.33	1.39
14	B	1236	CLA	C1B-CHB	-2.27	1.33	1.39
14	A	1106	CLA	C1B-CHB	-2.27	1.33	1.39
17	B	4009	BCR	C23-C22	-2.27	1.40	1.45
14	A	1122	CLA	MG-NB	2.27	2.10	2.05
14	B	1211	CLA	CHC-C1C	2.27	1.43	1.35
14	A	1133	CLA	C3B-C2B	-2.26	1.37	1.41
14	A	1118	CLA	CHB-C4A	2.26	1.41	1.36
17	B	4017	BCR	C23-C22	-2.26	1.40	1.45
14	B	1236	CLA	C3D-CAD	-2.27	1.42	1.47
14	B	1231	CLA	CHB-C4A	2.26	1.41	1.36
17	A	4008	BCR	C26-C25	2.26	1.37	1.34
14	B	1012	CLA	MG-NC	2.26	2.13	2.07
14	J	1302	CLA	CAA-C2A	2.26	1.58	1.54
14	B	1236	CLA	CHC-C1C	2.26	1.43	1.35
15	B	2002	PQN	C5-C4	-2.26	1.43	1.48
14	A	1105	CLA	CHB-C4A	2.26	1.41	1.36
14	B	1231	CLA	CBA-CGA	-2.26	1.48	1.49
14	A	1119	CLA	MG-NB	2.25	2.10	2.05
14	A	1140	CLA	C3D-CAD	-2.25	1.42	1.47
17	B	4014	BCR	C23-C22	-2.25	1.40	1.45
14	B	1021	CLA	CHB-C4A	2.25	1.41	1.36
14	A	1125	CLA	C1C-NC	-2.25	1.36	1.38
14	B	1209	CLA	C1C-NC	-2.25	1.36	1.38
14	K	1401	CLA	CHC-C1C	2.25	1.43	1.35
14	A	1011	CLA	CHB-C4A	2.24	1.41	1.36
14	B	1219	CLA	CHB-C4A	2.24	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1213	CLA	CHC-C1C	2.24	1.43	1.35
14	A	1109	CLA	CAA-C2A	2.24	1.58	1.54
14	A	1128	CLA	C1B-NB	2.24	1.37	1.34
17	L	4019	BCR	C2-C1	2.24	1.59	1.54
14	B	1227	CLA	CAA-C2A	2.24	1.58	1.54
17	B	4005	BCR	C29-C30	2.24	1.59	1.54
14	A	1133	CLA	CHB-C4A	2.24	1.41	1.36
17	I	4018	BCR	C2-C1	2.24	1.59	1.54
14	A	1138	CLA	C1B-CHB	-2.24	1.33	1.39
14	B	1222	CLA	CAA-C2A	2.24	1.58	1.54
17	I	4018	BCR	C33-C5	2.24	1.54	1.51
14	B	1221	CLA	C1B-CHB	-2.23	1.33	1.39
14	B	1231	CLA	CAA-C2A	2.23	1.58	1.54
14	B	1206	CLA	MG-NC	2.23	2.13	2.07
14	A	1113	CLA	C1C-NC	-2.23	1.36	1.38
14	A	1126	CLA	C4B-NB	2.23	1.37	1.34
14	A	1102	CLA	C3D-CAD	-2.23	1.42	1.47
14	B	1210	CLA	MG-NC	2.23	2.13	2.07
14	B	1216	CLA	CHC-C1C	2.23	1.43	1.35
14	A	1107	CLA	CHC-C1C	2.22	1.43	1.35
14	B	1208	CLA	CHC-C1C	2.22	1.43	1.35
14	A	1128	CLA	CAA-C2A	2.22	1.58	1.54
14	A	1101	CLA	C4A-NA	-2.22	1.34	1.39
14	A	1116	CLA	C5-C3	2.22	1.56	1.51
14	B	1224	CLA	C1A-NA	2.21	1.37	1.32
14	A	1139	CLA	C4B-NB	2.21	1.37	1.34
14	A	1402	CLA	CAA-C2A	2.21	1.58	1.54
14	A	1136	CLA	CAA-C2A	2.21	1.58	1.54
14	A	1115	CLA	C3B-C2B	-2.21	1.37	1.41
14	A	1117	CLA	C1-C2	2.21	1.56	1.49
17	L	4022	BCR	C5-C6	2.21	1.37	1.34
14	B	1204	CLA	CHB-C4A	2.20	1.41	1.36
14	L	1501	CLA	C3D-CAD	-2.20	1.42	1.47
14	B	1239	CLA	CHB-C4A	2.20	1.41	1.36
14	B	1201	CLA	CAA-C2A	2.20	1.58	1.54
14	A	1133	CLA	C5-C3	2.20	1.56	1.51
17	B	4010	BCR	C29-C30	2.20	1.59	1.54
14	F	1301	CLA	MG-NC	2.20	2.13	2.07
14	B	1211	CLA	C3B-C2B	-2.20	1.37	1.41
14	B	1226	CLA	OBD-CAD	2.19	1.25	1.22
14	A	1112	CLA	CAA-C2A	2.20	1.58	1.54
14	A	1118	CLA	C3D-CAD	-2.19	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1217	CLA	C1C-NC	-2.19	1.36	1.38
14	A	1128	CLA	C5-C3	2.19	1.56	1.51
17	I	4020	BCR	C19-C18	-2.19	1.41	1.45
15	A	2001	PQN	C9-C10	2.19	1.43	1.39
14	A	1011	CLA	CHC-C1C	2.19	1.42	1.35
14	B	1233	CLA	C3B-C2B	-2.19	1.37	1.41
14	B	1213	CLA	C4-C3	2.19	1.56	1.50
14	A	1113	CLA	CHC-C1C	2.18	1.42	1.35
14	A	1114	CLA	C3B-C2B	-2.18	1.37	1.41
14	A	1129	CLA	MG-NB	2.19	2.09	2.05
14	B	1233	CLA	CHC-C1C	2.18	1.42	1.35
14	F	1301	CLA	CHB-C4A	2.18	1.41	1.36
14	B	1227	CLA	C4A-NA	-2.18	1.34	1.39
14	A	1112	CLA	C1B-CHB	-2.18	1.33	1.39
14	A	1101	CLA	C1B-CHB	-2.18	1.33	1.39
14	A	1115	CLA	C1B-NB	2.18	1.37	1.34
14	A	1137	CLA	CHB-C4A	2.18	1.41	1.36
14	A	1135	CLA	MG-NC	2.18	2.13	2.07
14	B	1239	CLA	C3B-C2B	-2.18	1.37	1.41
14	B	1220	CLA	C3B-C2B	-2.18	1.37	1.41
14	B	1235	CLA	C1B-CHB	-2.18	1.33	1.39
14	B	1210	CLA	CHC-C1C	2.18	1.42	1.35
14	A	1101	CLA	CHC-C1C	2.18	1.42	1.35
17	A	4003	BCR	C29-C30	2.18	1.59	1.54
14	A	1118	CLA	C5-C3	2.17	1.56	1.51
14	A	1132	CLA	C1B-CHB	-2.17	1.33	1.39
14	M	1601	CLA	C1C-NC	-2.17	1.36	1.38
14	A	1137	CLA	C1C-NC	-2.17	1.36	1.38
14	B	1225	CLA	C1C-NC	-2.17	1.36	1.38
17	L	4019	BCR	C38-C26	2.17	1.54	1.51
17	J	4015	BCR	C26-C25	2.17	1.37	1.34
14	A	1237	CLA	C3D-CAD	-2.17	1.42	1.47
17	A	4007	BCR	C26-C25	2.16	1.37	1.34
14	B	1212	CLA	C3D-CAD	-2.16	1.42	1.47
14	B	1226	CLA	C4A-NA	-2.16	1.34	1.39
14	B	1205	CLA	CHC-C1C	2.16	1.42	1.35
14	A	1110	CLA	MG-NB	2.16	2.09	2.05
14	B	1222	CLA	C4A-NA	-2.16	1.34	1.39
14	A	1110	CLA	CHB-C4A	2.15	1.41	1.36
14	L	1502	CLA	C1C-NC	-2.15	1.36	1.38
14	A	1111	CLA	C3D-CAD	-2.15	1.43	1.47
17	B	4017	BCR	C26-C25	2.15	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1204	CLA	C4A-NA	-2.15	1.34	1.39
14	B	1230	CLA	CHC-C1C	2.15	1.42	1.35
17	I	4020	BCR	C33-C5	2.15	1.54	1.51
14	A	1133	CLA	CHC-C1C	2.15	1.42	1.35
14	A	1136	CLA	C1B-CHB	-2.15	1.33	1.39
14	A	1123	CLA	C3D-CAD	-2.15	1.43	1.47
15	A	2001	PQN	C5-C4	-2.14	1.43	1.48
14	B	1203	CLA	CAA-C2A	2.14	1.57	1.54
14	A	1111	CLA	C1B-CHB	-2.14	1.33	1.39
14	A	1013	CLA	CHC-C1C	2.14	1.42	1.35
14	A	1123	CLA	C1C-NC	-2.14	1.36	1.38
14	A	1022	CLA	MG-NC	2.14	2.13	2.07
14	B	1232	CLA	C1B-CHB	-2.14	1.34	1.39
14	A	1114	CLA	CHC-C1C	2.14	1.42	1.35
14	B	1226	CLA	C1B-NB	2.14	1.37	1.34
14	B	1210	CLA	C1B-CHB	-2.14	1.34	1.39
14	B	1218	CLA	CAA-C2A	2.14	1.57	1.54
14	A	1103	CLA	C1B-CHB	-2.14	1.34	1.39
14	B	1201	CLA	C4A-NA	-2.14	1.34	1.39
14	A	1115	CLA	CAA-C2A	2.14	1.57	1.54
14	B	1235	CLA	C1A-NA	2.14	1.36	1.32
14	A	1104	CLA	C3D-CAD	-2.14	1.43	1.47
14	A	1103	CLA	CHB-C4A	2.14	1.41	1.36
17	M	4021	BCR	C26-C25	2.13	1.37	1.34
14	A	1121	CLA	CHC-C1C	2.13	1.42	1.35
17	L	4022	BCR	C23-C22	-2.13	1.41	1.45
14	A	1013	CLA	C4A-NA	-2.13	1.34	1.39
14	B	1225	CLA	C1A-NA	2.13	1.36	1.32
14	A	1111	CLA	CHC-C1C	2.13	1.42	1.35
14	A	1132	CLA	MG-NB	2.13	2.09	2.05
14	A	1132	CLA	C3D-CAD	-2.13	1.43	1.47
14	B	1232	CLA	C4A-NA	-2.13	1.34	1.39
14	A	1118	CLA	C4A-NA	-2.13	1.34	1.39
14	A	1104	CLA	C4A-NA	-2.13	1.34	1.39
14	B	1211	CLA	C3D-CAD	-2.13	1.43	1.47
14	A	1115	CLA	C1B-CHB	-2.12	1.34	1.39
14	A	1129	CLA	C4-C3	2.12	1.55	1.48
14	A	1109	CLA	C1B-CHB	-2.12	1.34	1.39
14	B	1204	CLA	MG-NB	2.12	2.09	2.05
14	A	1134	CLA	C3B-C2B	-2.12	1.37	1.41
14	A	1124	CLA	C4B-NB	2.12	1.37	1.34
14	B	1202	CLA	CHB-C4A	2.12	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1221	CLA	CAA-C2A	2.12	1.57	1.54
14	B	1231	CLA	C4A-NA	-2.12	1.34	1.39
14	A	1122	CLA	C1B-CHB	-2.11	1.34	1.39
14	B	1216	CLA	C1B-CHB	-2.11	1.34	1.39
17	I	4018	BCR	C19-C18	-2.11	1.41	1.45
15	B	2002	PQN	C10-C1	-2.11	1.44	1.48
14	B	1236	CLA	C4A-NA	-2.11	1.34	1.39
14	A	1104	CLA	MG-ND	-2.11	2.00	2.05
14	A	1107	CLA	C3B-CAB	-2.10	1.47	1.49
14	F	1301	CLA	C3B-C2B	-2.10	1.37	1.41
14	A	1114	CLA	C3D-CAD	-2.10	1.43	1.47
15	A	2001	PQN	C8-C7	2.10	1.44	1.37
14	L	1503	CLA	C1C-NC	-2.10	1.36	1.38
14	B	1225	CLA	C1-C2	2.10	1.56	1.49
14	B	1231	CLA	C1B-CHB	-2.10	1.34	1.39
14	B	1230	CLA	C4A-NA	-2.10	1.34	1.39
14	A	1125	CLA	C3D-CAD	-2.10	1.43	1.47
14	A	1106	CLA	C4A-NA	-2.10	1.34	1.39
14	B	1227	CLA	C1B-CHB	-2.09	1.34	1.39
14	B	1222	CLA	CHC-C1C	2.09	1.42	1.35
14	A	1109	CLA	CHC-C1C	2.09	1.42	1.35
14	B	1212	CLA	C1C-NC	-2.09	1.36	1.38
14	B	1218	CLA	CHB-C4A	2.09	1.41	1.36
14	J	1302	CLA	C3B-C2B	-2.09	1.37	1.41
14	B	1212	CLA	CAA-C2A	2.09	1.57	1.54
17	B	4005	BCR	C5-C6	2.08	1.37	1.34
14	A	1801	CLA	C4-C3	2.09	1.56	1.50
14	A	1139	CLA	C1C-NC	-2.08	1.36	1.38
14	B	1203	CLA	C4A-NA	-2.08	1.34	1.39
17	A	4008	BCR	C33-C5	2.08	1.54	1.51
14	A	1013	CLA	C2-C3	2.08	1.37	1.32
17	A	4007	BCR	C14-C13	2.08	1.38	1.35
14	B	1226	CLA	MG-NB	2.08	2.09	2.05
14	A	1126	CLA	C4-C3	2.08	1.56	1.50
14	A	1127	CLA	MG-NC	2.08	2.13	2.07
14	B	1232	CLA	C3B-CAB	2.07	1.51	1.49
14	A	1132	CLA	C2-C3	2.08	1.37	1.32
14	B	1211	CLA	C1B-CHB	-2.07	1.34	1.39
15	A	2001	PQN	C11-C3	2.07	1.55	1.51
14	A	1138	CLA	C4A-NA	-2.07	1.34	1.39
17	I	4020	BCR	C14-C13	2.07	1.38	1.35
14	A	1133	CLA	CAA-C2A	2.07	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1108	CLA	MG-NC	2.07	2.13	2.07
14	B	1228	CLA	CAA-C2A	2.07	1.57	1.54
14	A	1402	CLA	CHC-C1C	2.07	1.42	1.35
14	B	1023	CLA	C4-C3	2.07	1.56	1.50
17	A	4003	BCR	C5-C6	2.06	1.37	1.34
14	A	1127	CLA	C4A-NA	-2.06	1.34	1.39
14	B	1238	CLA	MG-NB	2.06	2.09	2.05
14	A	1107	CLA	C3D-CAD	-2.06	1.43	1.47
14	A	1133	CLA	MG-NB	2.05	2.09	2.05
14	L	1502	CLA	C3B-C2B	-2.05	1.37	1.41
14	A	1127	CLA	CHC-C1C	2.05	1.42	1.35
14	K	1401	CLA	C1B-CHB	-2.05	1.34	1.39
14	A	1117	CLA	C4A-NA	-2.05	1.34	1.39
17	A	4008	BCR	C19-C18	-2.05	1.41	1.45
14	B	1239	CLA	CAA-CBA	-2.05	1.45	1.52
14	B	1227	CLA	C3D-CAD	-2.04	1.43	1.47
14	A	1140	CLA	CAA-C2A	2.04	1.57	1.54
14	A	1112	CLA	C1C-NC	-2.04	1.36	1.38
14	A	1114	CLA	CAA-C2A	2.04	1.57	1.54
14	A	1022	CLA	C1B-CHB	-2.04	1.34	1.39
14	B	1201	CLA	C3B-C2B	-2.04	1.37	1.41
14	B	1204	CLA	C4B-NB	2.04	1.37	1.34
14	A	1011	CLA	C4D-CHA	2.03	1.47	1.39
14	A	1126	CLA	C1B-CHB	-2.03	1.34	1.39
14	B	1211	CLA	C4A-NA	-2.04	1.34	1.39
14	A	1120	CLA	CAA-C2A	2.03	1.57	1.54
14	A	1125	CLA	C3B-C2B	-2.03	1.37	1.41
14	A	1104	CLA	CHB-C4A	2.03	1.41	1.36
14	A	1111	CLA	C4A-NA	-2.03	1.34	1.39
14	B	1021	CLA	MG-NC	2.03	2.13	2.07
14	A	1120	CLA	C4A-NA	-2.03	1.34	1.39
14	A	1140	CLA	OBD-CAD	2.03	1.25	1.22
14	B	1230	CLA	C4-C3	2.03	1.55	1.50
17	A	4003	BCR	C24-C23	2.03	1.38	1.32
14	B	1221	CLA	C3D-CAD	-2.03	1.43	1.47
14	A	1801	CLA	C5-C3	2.03	1.56	1.51
14	A	1108	CLA	CHC-C1C	2.03	1.42	1.35
14	A	1120	CLA	CHB-C4A	2.03	1.41	1.36
17	A	4008	BCR	C2-C1	2.02	1.59	1.54
14	A	1237	CLA	C1B-CHB	-2.02	1.34	1.39
14	B	1205	CLA	CAA-C2A	2.02	1.57	1.54
14	B	1201	CLA	C3D-CAD	-2.02	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1601	CLA	C3D-CAD	-2.02	1.43	1.47
14	A	1126	CLA	C4A-NA	-2.02	1.34	1.39
14	A	1013	CLA	C1A-NA	2.02	1.36	1.32
14	A	1801	CLA	C1B-CHB	-2.02	1.34	1.39
14	B	1212	CLA	C1B-CHB	-2.02	1.34	1.39
14	A	1110	CLA	C4-C3	2.02	1.55	1.50
14	B	1211	CLA	C5-C3	2.02	1.56	1.51
14	B	1234	CLA	C4-C3	2.02	1.55	1.50
14	A	1402	CLA	C3B-C2B	-2.01	1.37	1.41
14	A	1110	CLA	CHC-C1C	2.01	1.42	1.35
14	A	1113	CLA	CAA-C2A	2.01	1.57	1.54
14	B	1222	CLA	CHB-C4A	2.01	1.41	1.36
14	A	1122	CLA	C3D-CAD	-2.01	1.43	1.47
18	A	5001	LHG	O7-C5	-2.01	1.41	1.46
14	B	1225	CLA	C1B-NB	2.01	1.37	1.34
14	A	1130	CLA	C3D-CAD	-2.01	1.43	1.47
14	L	1501	CLA	CHB-C4A	2.00	1.41	1.36
14	B	1215	CLA	C1C-NC	-2.00	1.36	1.38
14	B	1226	CLA	C1C-NC	-2.00	1.36	1.38
15	B	2002	PQN	C8-C7	2.00	1.43	1.37

All (1874) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1011	CLA	CBD-CHA-C1A	9.87	141.67	128.77
15	A	2001	PQN	C14-C13-C15	8.13	127.76	115.39
15	B	2002	PQN	C11-C12-C13	-8.06	113.14	126.76
15	A	2001	PQN	C11-C12-C13	-7.95	113.34	126.76
14	A	1011	CLA	C4D-CHA-CBD	-7.82	90.95	109.37
15	A	2001	PQN	C15-C13-C12	-7.62	106.41	121.08
14	A	1011	CLA	O2D-CGD-CBD	7.43	126.47	111.33
15	B	2002	PQN	C14-C13-C15	6.98	126.01	115.39
18	A	5003	LHG	O8-C23-C24	6.86	120.59	111.94
15	B	2002	PQN	C15-C13-C12	-6.48	108.62	121.08
14	B	1023	CLA	C2B-C3B-CAB	-6.37	114.30	127.33
14	A	1011	CLA	C3D-CAD-CBD	-6.23	98.79	107.60
14	A	1129	CLA	C2B-C3B-CAB	-6.05	114.94	127.33
14	A	1022	CLA	C2B-C3B-CAB	-6.02	115.00	127.33
14	A	1402	CLA	CHA-CBD-CAD	-5.98	104.19	109.72
17	B	4004	BCR	C38-C26-C25	5.92	131.22	124.51
14	J	1303	CLA	CHA-CBD-CAD	-5.86	104.30	109.72
14	B	1224	CLA	C2B-C3B-CAB	-5.84	115.37	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1132	CLA	C2B-C3B-CAB	-5.79	115.48	127.33
18	A	5001	LHG	C25-C24-C23	5.78	136.18	113.51
14	L	1501	CLA	C2B-C3B-CAB	-5.76	115.53	127.33
14	A	1128	CLA	C2B-C3B-CAB	-5.73	115.60	127.33
14	B	1204	CLA	C2B-C3B-CAB	-5.73	115.60	127.33
19	B	5002	LMG	C30-C29-C28	5.73	135.97	113.51
17	B	4005	BCR	C38-C26-C25	5.71	130.99	124.51
14	B	1221	CLA	C2B-C3B-CAB	-5.68	115.70	127.33
14	B	1235	CLA	C2B-C3B-CAB	-5.60	115.87	127.33
14	A	1104	CLA	CAA-C2A-C3A	-5.58	99.84	113.04
14	B	1227	CLA	C2B-C3B-CAB	-5.53	116.02	127.33
14	A	1123	CLA	C2B-C3B-CAB	-5.52	116.04	127.33
14	B	1229	CLA	C2B-C3B-CAB	-5.50	116.06	127.33
17	A	4008	BCR	C38-C26-C25	5.44	130.68	124.51
14	A	1106	CLA	C2B-C3B-CAB	-5.42	116.24	127.33
14	A	1801	CLA	C2B-C3B-CAB	-5.39	116.29	127.33
14	B	1228	CLA	C2B-C3B-CAB	-5.37	116.34	127.33
14	B	1232	CLA	C2B-C3B-CAB	-5.35	116.38	127.33
14	B	1231	CLA	C2B-C3B-CAB	-5.35	116.38	127.33
14	A	1128	CLA	C4B-C3B-CAB	5.34	137.99	127.18
14	A	1125	CLA	C2B-C3B-CAB	-5.32	116.44	127.33
14	A	1136	CLA	C2B-C3B-CAB	-5.28	116.53	127.33
14	B	1208	CLA	C2B-C3B-CAB	-5.27	116.54	127.33
14	A	1011	CLA	O1D-CGD-CBD	-5.26	113.64	124.42
14	L	1502	CLA	C2B-C3B-CAB	-5.24	116.61	127.33
14	A	1120	CLA	C2B-C3B-CAB	-5.23	116.62	127.33
14	B	1012	CLA	C2B-C3B-CAB	-5.23	116.63	127.33
14	B	1214	CLA	C2B-C3B-CAB	-5.23	116.63	127.33
14	B	1220	CLA	C2B-C3B-CAB	-5.18	116.72	127.33
14	B	1232	CLA	C4B-C3B-CAB	5.16	137.63	127.18
14	B	1212	CLA	C2B-C3B-CAB	-5.13	116.82	127.33
14	A	1101	CLA	C2B-C3B-CAB	-5.13	116.83	127.33
14	B	1218	CLA	C2B-C3B-CAB	-5.12	116.85	127.33
17	L	4022	BCR	C33-C5-C6	5.11	130.31	124.51
14	A	1112	CLA	C2B-C3B-CAB	-5.11	116.87	127.33
14	A	1121	CLA	C2B-C3B-CAB	-5.11	116.87	127.33
17	A	4001	BCR	C38-C26-C25	5.09	130.28	124.51
14	A	1115	CLA	C2B-C3B-CAB	-5.09	116.92	127.33
14	B	1230	CLA	C2B-C3B-CAB	-5.09	116.91	127.33
14	A	1107	CLA	C2B-C3B-CAB	-5.07	116.94	127.33
14	A	1237	CLA	C2B-C3B-CAB	-5.06	116.97	127.33
14	B	1211	CLA	C2B-C3B-CAB	-5.04	117.00	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	4014	BCR	C33-C5-C6	5.04	130.22	124.51
14	A	1138	CLA	C2B-C3B-CAB	-5.04	117.02	127.33
14	A	1118	CLA	C2B-C3B-CAB	-5.04	117.02	127.33
14	B	1233	CLA	C2B-C3B-CAB	-5.03	117.03	127.33
14	B	1225	CLA	C2B-C3B-CAB	-5.02	117.05	127.33
17	J	4012	BCR	C38-C26-C25	5.02	130.20	124.51
14	B	1213	CLA	C2B-C3B-CAB	-5.00	117.11	127.33
14	B	1234	CLA	C2B-C3B-CAB	-4.98	117.13	127.33
14	L	1503	CLA	C2B-C3B-CAB	-4.97	117.16	127.33
14	A	1116	CLA	C2B-C3B-CAB	-4.92	117.25	127.33
14	A	1105	CLA	C2B-C3B-CAB	-4.91	117.29	127.33
14	A	1134	CLA	C2B-C3B-CAB	-4.90	117.31	127.33
14	B	1216	CLA	C2B-C3B-CAB	-4.89	117.31	127.33
14	B	1229	CLA	C4B-C3B-CAB	4.87	137.05	127.18
17	L	4019	BCR	C33-C5-C6	4.86	130.02	124.51
14	J	1302	CLA	C2B-C3B-CAB	-4.86	117.38	127.33
14	J	1303	CLA	C2B-C3B-CAB	-4.81	117.48	127.33
14	A	1106	CLA	C4B-C3B-CAB	4.81	136.92	127.18
14	A	1110	CLA	C2B-C3B-CAB	-4.81	117.49	127.33
14	A	1101	CLA	C4B-C3B-CAB	4.80	136.90	127.18
14	A	1114	CLA	C2B-C3B-CAB	-4.75	117.60	127.33
14	B	1231	CLA	C4B-C3B-CAB	4.74	136.78	127.18
14	A	1137	CLA	C2B-C3B-CAB	-4.74	117.63	127.33
17	J	4015	BCR	C33-C5-C6	4.74	129.88	124.51
14	L	1501	CLA	C4B-C3B-CAB	4.74	136.77	127.18
14	B	1209	CLA	C2B-C3B-CAB	-4.73	117.66	127.33
17	B	4006	BCR	C33-C5-C6	4.71	129.85	124.51
14	A	1123	CLA	C4B-C3B-CAB	4.68	136.65	127.18
14	A	1129	CLA	C4B-C3B-CAB	4.66	136.62	127.18
14	B	1221	CLA	C4B-C3B-CAB	4.66	136.61	127.18
14	A	1801	CLA	C4B-C3B-CAB	4.66	136.61	127.18
14	A	1011	CLA	CGD-CBD-CHA	4.65	126.77	110.96
14	B	1205	CLA	C2B-C3B-CAB	-4.65	117.81	127.33
14	F	1301	CLA	C2B-C3B-CAB	-4.65	117.82	127.33
17	B	4010	BCR	C33-C5-C6	4.65	129.78	124.51
14	A	1108	CLA	C2B-C3B-CAB	-4.63	117.85	127.33
14	B	1204	CLA	C4B-C3B-CAB	4.62	136.54	127.18
14	A	1104	CLA	O2A-CGA-CBA	4.62	126.48	111.94
17	I	4018	BCR	C33-C5-C6	4.62	129.75	124.51
17	B	4004	BCR	C33-C5-C6	4.62	129.74	124.51
14	B	1228	CLA	C4B-C3B-CAB	4.61	136.52	127.18
14	A	1112	CLA	C4B-C3B-CAB	4.60	136.49	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1125	CLA	C4B-C3B-CAB	4.60	136.49	127.18
14	K	1401	CLA	C2B-C3B-CAB	-4.60	117.92	127.33
14	B	1201	CLA	C2B-C3B-CAB	-4.59	117.93	127.33
14	A	1119	CLA	CMB-C2B-C1B	-4.57	121.58	128.62
14	B	1021	CLA	C2B-C3B-CAB	-4.57	117.97	127.33
14	A	1022	CLA	C4B-C3B-CAB	4.57	136.43	127.18
17	J	4015	BCR	C38-C26-C25	4.57	129.69	124.51
14	A	1122	CLA	C2B-C3B-CAB	-4.57	117.98	127.33
14	A	1140	CLA	C2B-C3B-CAB	-4.57	117.98	127.33
14	A	1120	CLA	C4B-C3B-CAB	4.56	136.41	127.18
14	B	1235	CLA	C4B-C3B-CAB	4.55	136.39	127.18
14	M	1601	CLA	C2B-C3B-CAB	-4.55	118.01	127.33
17	A	4003	BCR	C38-C26-C25	4.53	129.65	124.51
14	X	1701	CLA	C2B-C3B-CAB	-4.53	118.06	127.33
14	B	1236	CLA	C2B-C3B-CAB	-4.53	118.06	127.33
14	B	1218	CLA	C4B-C3B-CAB	4.52	136.33	127.18
14	A	1117	CLA	CMB-C2B-C1B	-4.52	121.67	128.62
14	J	1303	CLA	OBD-CAD-C3D	4.51	130.75	123.74
14	B	1208	CLA	C4B-C3B-CAB	4.50	136.29	127.18
14	B	1215	CLA	CMB-C2B-C1B	-4.50	121.70	128.62
14	A	1121	CLA	C4B-C3B-CAB	4.49	136.27	127.18
14	A	1133	CLA	C2B-C3B-CAB	-4.49	118.15	127.33
17	B	4006	BCR	C7-C8-C9	4.49	132.93	126.22
14	B	1233	CLA	C4B-C3B-CAB	4.48	136.25	127.18
14	B	1234	CLA	C4B-C3B-CAB	4.47	136.24	127.18
14	B	1224	CLA	C4B-C3B-CAB	4.47	136.23	127.18
17	L	4022	BCR	C38-C26-C25	4.47	129.57	124.51
14	A	1011	CLA	C2B-C3B-CAB	-4.46	118.19	127.33
14	A	1118	CLA	C4B-C3B-CAB	4.46	136.21	127.18
14	B	1023	CLA	C4B-C3B-CAB	4.45	136.19	127.18
14	B	1217	CLA	C2B-C3B-CAB	-4.45	118.22	127.33
14	A	1402	CLA	C2B-C3B-CAB	-4.45	118.22	127.33
14	B	1236	CLA	C1-O2A-CGA	4.45	120.28	115.06
17	F	4016	BCR	C38-C26-C25	4.45	129.55	124.51
14	A	1109	CLA	C2B-C3B-CAB	-4.44	118.23	127.33
14	A	1138	CLA	C4B-C3B-CAB	4.44	136.16	127.18
14	B	1212	CLA	C4B-C3B-CAB	4.43	136.14	127.18
14	A	1115	CLA	C4B-C3B-CAB	4.42	136.13	127.18
14	A	1105	CLA	C4B-C3B-CAB	4.42	136.13	127.18
17	A	4002	BCR	C38-C26-C25	4.41	129.51	124.51
14	A	1136	CLA	C4B-C3B-CAB	4.40	136.09	127.18
17	I	4018	BCR	C38-C26-C25	4.39	129.49	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	4014	BCR	C38-C26-C25	4.37	129.46	124.51
14	B	1224	CLA	O2A-CGA-CBA	4.36	125.66	111.94
14	L	1502	CLA	C4B-C3B-CAB	4.35	135.99	127.18
14	B	1211	CLA	C4B-C3B-CAB	4.35	135.99	127.18
17	M	4021	BCR	C38-C26-C25	4.34	129.43	124.51
14	B	1207	CLA	C2B-C3B-CAB	-4.33	118.46	127.33
14	A	1102	CLA	C10-C11-C12	-4.33	106.11	114.68
14	A	1134	CLA	C4B-C3B-CAB	4.32	135.93	127.18
14	A	1139	CLA	C2B-C3B-CAB	-4.32	118.48	127.33
17	A	4011	BCR	C7-C8-C9	4.32	132.68	126.22
14	A	1102	CLA	C2B-C3B-CAB	-4.31	118.50	127.33
14	A	1116	CLA	C4B-C3B-CAB	4.31	135.90	127.18
14	B	1220	CLA	C4B-C3B-CAB	4.30	135.89	127.18
14	A	1237	CLA	C4B-C3B-CAB	4.29	135.86	127.18
17	A	4001	BCR	C33-C5-C6	4.28	129.36	124.51
14	B	1216	CLA	C4B-C3B-CAB	4.28	135.84	127.18
17	A	4003	BCR	C33-C5-C6	4.27	129.35	124.51
17	A	4007	BCR	C38-C26-C25	4.26	129.34	124.51
14	A	1402	CLA	OBD-CAD-C3D	4.26	130.35	123.74
14	B	1214	CLA	C4B-C3B-CAB	4.26	135.80	127.18
17	B	4006	BCR	C38-C26-C25	4.23	129.30	124.51
14	B	1012	CLA	O2D-CGD-CBD	4.23	119.94	111.33
14	J	1303	CLA	C4B-C3B-CAB	4.22	135.73	127.18
14	B	1227	CLA	C4B-C3B-CAB	4.21	135.70	127.18
14	A	1132	CLA	O2D-CGD-CBD	4.21	119.91	111.33
14	B	1226	CLA	O2D-CGD-CBD	4.21	119.90	111.33
14	B	1213	CLA	C4B-C3B-CAB	4.20	135.68	127.18
14	J	1302	CLA	C4B-C3B-CAB	4.19	135.67	127.18
17	L	4019	BCR	C38-C26-C25	4.18	129.25	124.51
14	A	1114	CLA	C4B-C3B-CAB	4.18	135.64	127.18
14	A	1110	CLA	C4B-C3B-CAB	4.18	135.64	127.18
14	B	1209	CLA	C4B-C3B-CAB	4.18	135.64	127.18
14	B	1201	CLA	C4B-C3B-CAB	4.17	135.62	127.18
14	K	1401	CLA	C4B-C3B-CAB	4.17	135.61	127.18
14	B	1226	CLA	CMB-C2B-C1B	-4.15	122.23	128.62
14	A	1108	CLA	C4B-C3B-CAB	4.15	135.58	127.18
14	B	1217	CLA	C4A-NA-C1A	4.15	112.24	106.52
14	F	1301	CLA	C4B-C3B-CAB	4.15	135.57	127.18
14	A	1130	CLA	C4A-NA-C1A	4.13	112.21	106.52
14	A	1127	CLA	CMB-C2B-C1B	-4.13	122.27	128.62
14	B	1205	CLA	C4B-C3B-CAB	4.12	135.53	127.18
17	B	4009	BCR	C38-C26-C25	4.12	129.18	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1238	CLA	C2B-C3B-CAB	-4.11	118.92	127.33
14	M	1601	CLA	C4A-NA-C1A	4.11	112.18	106.52
14	B	1201	CLA	O2D-CGD-CBD	4.11	119.70	111.33
14	B	1012	CLA	C4B-C3B-CAB	4.10	135.49	127.18
17	B	4005	BCR	C33-C5-C6	4.10	129.16	124.51
14	X	1701	CLA	C4B-C3B-CAB	4.09	135.45	127.18
17	A	4011	BCR	C33-C5-C6	4.08	129.13	124.51
14	M	1601	CLA	C4B-C3B-CAB	4.07	135.43	127.18
14	A	1113	CLA	C4A-NA-C1A	4.05	112.10	106.52
17	I	4020	BCR	C24-C23-C22	4.04	132.26	126.22
14	L	1501	CLA	O2D-CGD-CBD	4.04	119.55	111.33
17	I	4020	BCR	C38-C26-C25	4.03	129.08	124.51
14	A	1135	CLA	O2A-CGA-CBA	4.03	124.62	111.94
17	J	4012	BCR	C33-C5-C6	4.03	129.08	124.51
17	A	4008	BCR	C38-C26-C27	-4.03	105.95	113.34
14	A	1118	CLA	C4A-NA-C1A	4.02	112.06	106.52
17	B	4006	BCR	C29-C30-C25	4.02	117.11	110.44
14	A	1013	CLA	O2A-CGA-CBA	4.01	124.56	111.94
14	B	1209	CLA	C4A-NA-C1A	4.00	112.04	106.52
14	A	1110	CLA	C4A-NA-C1A	4.00	112.04	106.52
14	A	1137	CLA	O2A-CGA-CBA	4.00	124.53	111.94
14	B	1217	CLA	C4B-C3B-CAB	3.99	135.26	127.18
14	B	1218	CLA	C4A-NA-C1A	3.99	112.03	106.52
14	A	1137	CLA	C4B-C3B-CAB	3.99	135.25	127.18
14	A	1011	CLA	C2D-C1D-ND	3.98	112.42	109.41
14	J	1302	CLA	C4A-NA-C1A	3.97	112.00	106.52
14	A	1119	CLA	CMB-C2B-C3B	3.96	131.20	124.97
14	A	1102	CLA	O2D-CGD-CBD	3.95	119.38	111.33
14	X	1701	CLA	C4A-NA-C1A	3.95	111.96	106.52
14	A	1801	CLA	C4A-NA-C1A	3.95	111.96	106.52
14	A	1133	CLA	C4B-C3B-CAB	3.95	135.17	127.18
14	B	1236	CLA	C4B-C3B-CAB	3.95	135.17	127.18
17	B	4005	BCR	C7-C8-C9	3.94	132.12	126.22
14	B	1233	CLA	C4A-NA-C1A	3.94	111.96	106.52
17	F	4016	BCR	C33-C5-C6	3.94	128.98	124.51
14	A	1402	CLA	C4B-C3B-CAB	3.94	135.16	127.18
14	A	1109	CLA	C4B-C3B-CAB	3.94	135.15	127.18
14	B	1225	CLA	O2A-CGA-CBA	3.93	124.32	111.94
14	B	1225	CLA	C4B-C3B-CAB	3.93	135.14	127.18
14	A	1132	CLA	C4B-C3B-CAB	3.93	135.14	127.18
14	A	1134	CLA	C4A-NA-C1A	3.93	111.94	106.52
17	B	4004	BCR	C38-C26-C27	-3.92	106.14	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4011	BCR	C38-C26-C25	3.92	128.95	124.51
14	B	1205	CLA	O2D-CGD-CBD	3.92	119.31	111.33
17	A	4002	BCR	C33-C5-C6	3.91	128.95	124.51
17	B	4010	BCR	C38-C26-C25	3.91	128.94	124.51
14	A	1107	CLA	C4B-C3B-CAB	3.91	135.10	127.18
14	B	1230	CLA	O2D-CGD-CBD	3.91	119.29	111.33
14	B	1230	CLA	C4B-C3B-CAB	3.90	135.08	127.18
14	A	1122	CLA	C4B-C3B-CAB	3.89	135.06	127.18
14	B	1227	CLA	C4A-NA-C1A	3.89	111.88	106.52
14	A	1140	CLA	C4B-C3B-CAB	3.88	135.03	127.18
14	A	1801	CLA	O2D-CGD-CBD	3.88	119.22	111.33
17	A	4011	BCR	C24-C23-C22	3.87	132.01	126.22
14	B	1239	CLA	C2B-C3B-CAB	-3.87	119.41	127.33
14	F	1301	CLA	C4A-NA-C1A	3.87	111.85	106.52
17	B	4017	BCR	C33-C5-C6	3.87	128.89	124.51
17	B	4017	BCR	C38-C26-C25	3.87	128.89	124.51
14	B	1211	CLA	O2D-CGD-CBD	3.86	119.20	111.33
14	L	1503	CLA	C4B-C3B-CAB	3.85	134.97	127.18
14	A	1114	CLA	C4A-NA-C1A	3.84	111.82	106.52
14	B	1021	CLA	C4B-C3B-CAB	3.84	134.96	127.18
14	A	1109	CLA	C4A-NA-C1A	3.84	111.82	106.52
14	A	1102	CLA	C4B-C3B-CAB	3.84	134.96	127.18
17	B	4014	BCR	C7-C8-C9	3.84	131.96	126.22
17	A	4007	BCR	C33-C5-C6	3.84	128.86	124.51
14	B	1223	CLA	CMB-C2B-C1B	-3.84	122.72	128.62
14	J	1303	CLA	C4A-NA-C1A	3.83	111.80	106.52
17	I	4018	BCR	C2-C1-C6	3.83	116.81	110.44
14	B	1230	CLA	C4A-NA-C1A	3.83	111.79	106.52
17	M	4021	BCR	C24-C23-C22	3.82	131.93	126.22
14	B	1215	CLA	C4A-NA-C1A	3.81	111.78	106.52
14	A	1120	CLA	C4A-NA-C1A	3.81	111.77	106.52
14	A	1140	CLA	O2A-CGA-CBA	3.81	123.93	111.94
14	B	1206	CLA	C2B-C3B-CAB	-3.81	119.54	127.33
14	A	1107	CLA	O2A-CGA-CBA	3.81	123.91	111.94
14	B	1219	CLA	C4A-NA-C1A	3.79	111.74	106.52
14	B	1205	CLA	O2A-CGA-CBA	3.79	123.86	111.94
14	B	1226	CLA	CMB-C2B-C3B	3.79	130.94	124.97
14	A	1104	CLA	CMB-C2B-C1B	-3.79	122.80	128.62
17	J	4015	BCR	C8-C7-C6	3.78	138.50	127.32
14	A	1107	CLA	C4A-NA-C1A	3.78	111.73	106.52
14	A	1139	CLA	C4B-C3B-CAB	3.78	134.82	127.18
14	A	1133	CLA	C4A-NA-C1A	3.77	111.72	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1120	CLA	O2A-CGA-CBA	3.77	123.81	111.94
14	A	1117	CLA	O2A-CGA-CBA	3.77	123.80	111.94
14	B	1204	CLA	C4A-NA-C1A	3.77	111.72	106.52
14	B	1215	CLA	O2A-CGA-CBA	3.76	123.78	111.94
14	A	1237	CLA	O2A-CGA-CBA	3.76	123.76	111.94
14	A	1117	CLA	C4A-NA-C1A	3.75	111.70	106.52
14	A	1129	CLA	C4A-NA-C1A	3.75	111.70	106.52
14	A	1111	CLA	C4A-NA-C1A	3.75	111.69	106.52
14	B	1212	CLA	O2D-CGD-CBD	3.75	118.96	111.33
14	B	1207	CLA	C4A-NA-C1A	3.75	111.68	106.52
14	B	1224	CLA	CBA-CAA-C2A	3.74	125.12	114.01
14	A	1118	CLA	O2A-CGA-CBA	3.74	123.71	111.94
14	B	1214	CLA	C10-C11-C12	-3.74	107.27	114.68
14	A	1801	CLA	O2A-CGA-CBA	3.74	123.71	111.94
14	B	1222	CLA	C4A-NA-C1A	3.74	111.67	106.52
14	B	1201	CLA	C4A-NA-C1A	3.73	111.67	106.52
17	B	4005	BCR	C24-C23-C22	3.71	131.77	126.22
14	A	1135	CLA	C4A-NA-C1A	3.71	111.63	106.52
14	A	1105	CLA	C4A-NA-C1A	3.71	111.63	106.52
14	B	1223	CLA	C4A-NA-C1A	3.71	111.63	106.52
14	B	1235	CLA	C4A-NA-C1A	3.71	111.63	106.52
14	A	1139	CLA	O2A-CGA-CBA	3.70	123.57	111.94
14	A	1402	CLA	C4A-NA-C1A	3.69	111.61	106.52
14	A	1106	CLA	C4A-NA-C1A	3.69	111.61	106.52
14	A	1122	CLA	C10-C11-C12	-3.69	107.38	114.68
14	A	1123	CLA	O2D-CGD-CBD	3.68	118.82	111.33
14	A	1102	CLA	C4A-NA-C1A	3.68	111.59	106.52
14	A	1113	CLA	O2D-CGD-CBD	3.67	118.81	111.33
14	A	1125	CLA	C4A-NA-C1A	3.67	111.58	106.52
17	B	4010	BCR	C7-C8-C9	3.67	131.71	126.22
17	B	4014	BCR	C33-C5-C4	-3.66	106.61	113.34
14	A	1138	CLA	C4A-NA-C1A	3.66	111.56	106.52
14	A	1109	CLA	C2D-C1D-ND	3.66	112.17	109.41
17	A	4011	BCR	C40-C30-C25	3.66	116.39	110.33
14	A	1125	CLA	O2D-CGD-CBD	3.66	118.78	111.33
17	B	4005	BCR	C38-C26-C27	-3.65	106.64	113.34
14	B	1222	CLA	O2D-CGD-CBD	3.65	118.77	111.33
14	B	1239	CLA	C4A-NA-C1A	3.65	111.55	106.52
14	B	1215	CLA	CMB-C2B-C3B	3.65	130.72	124.97
14	B	1206	CLA	CMB-C2B-C1B	-3.65	123.01	128.62
14	A	1121	CLA	O2A-CGA-CBA	3.65	123.42	111.94
14	A	1011	CLA	OBD-CAD-C3D	3.64	134.69	127.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1232	CLA	CMB-C2B-C1B	-3.64	123.02	128.62
17	A	4007	BCR	C24-C23-C22	3.64	131.66	126.22
14	B	1216	CLA	C4A-NA-C1A	3.64	111.53	106.52
14	A	1127	CLA	O2A-CGA-CBA	3.63	123.37	111.94
14	B	1212	CLA	C2D-C1D-ND	3.63	112.16	109.41
14	B	1207	CLA	C4B-C3B-CAB	3.63	134.53	127.18
17	M	4021	BCR	C33-C5-C6	3.63	128.62	124.51
14	B	1228	CLA	C4A-NA-C1A	3.63	111.52	106.52
14	A	1011	CLA	C4B-C3B-CAB	3.62	134.52	127.18
14	B	1217	CLA	O2A-CGA-CBA	3.62	123.34	111.94
14	B	1206	CLA	C4B-C3B-CAB	3.62	134.51	127.18
14	A	1116	CLA	C4A-NA-C1A	3.62	111.51	106.52
17	J	4013	BCR	C33-C5-C6	3.62	128.61	124.51
14	B	1212	CLA	C4A-NA-C1A	3.62	111.50	106.52
14	B	1012	CLA	OBD-CAD-CBD	-3.61	120.48	125.94
14	J	1303	CLA	C2A-C1A-CHA	3.61	127.29	123.57
14	B	1231	CLA	C4A-NA-C1A	3.61	111.50	106.52
14	A	1101	CLA	O2D-CGD-CBD	3.61	118.69	111.33
14	A	1124	CLA	C4A-NA-C1A	3.61	111.50	106.52
14	A	1022	CLA	OBD-CAD-CBD	-3.60	120.50	125.94
17	A	4003	BCR	C24-C23-C22	3.60	131.60	126.22
14	B	1210	CLA	CMB-C2B-C1B	-3.60	123.08	128.62
14	A	1103	CLA	CAA-C2A-C3A	-3.60	104.53	113.04
14	B	1214	CLA	C4A-NA-C1A	3.59	111.47	106.52
17	A	4003	BCR	C38-C26-C27	-3.59	106.74	113.34
14	A	1106	CLA	O2D-CGD-CBD	3.59	118.64	111.33
14	A	1124	CLA	CMB-C2B-C1B	-3.59	123.10	128.62
14	B	1211	CLA	C4A-NA-C1A	3.59	111.47	106.52
14	B	1211	CLA	C1-C2-C3	3.58	132.56	126.19
14	B	1214	CLA	O2A-CGA-CBA	3.58	123.21	111.94
14	B	1021	CLA	C4A-NA-C1A	3.58	111.45	106.52
17	I	4020	BCR	C33-C5-C6	3.57	128.56	124.51
17	J	4015	BCR	C24-C23-C22	3.57	131.56	126.22
14	A	1801	CLA	C1-C2-C3	3.57	132.53	126.19
14	A	1101	CLA	C4A-NA-C1A	3.57	111.44	106.52
17	A	4001	BCR	C38-C26-C27	-3.56	106.80	113.34
14	A	1116	CLA	O2A-CGA-CBA	3.56	123.13	111.94
14	A	1110	CLA	O2A-CGA-CBA	3.55	123.12	111.94
17	J	4012	BCR	C38-C26-C27	-3.55	106.81	113.34
14	A	1128	CLA	O2D-CGD-CBD	3.55	118.57	111.33
14	B	1202	CLA	C2D-C1D-ND	3.54	112.09	109.41
17	A	4008	BCR	C33-C5-C6	3.54	128.53	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1229	CLA	C4A-NA-C1A	3.54	111.40	106.52
14	B	1220	CLA	C4A-NA-C1A	3.54	111.40	106.52
14	M	1601	CLA	O2D-CGD-CBD	3.54	118.54	111.33
14	A	1122	CLA	C4A-NA-C1A	3.54	111.39	106.52
17	J	4015	BCR	C2-C1-C6	3.53	116.31	110.44
17	B	4006	BCR	C38-C26-C27	-3.53	106.86	113.34
17	B	4005	BCR	C30-C25-C26	-3.53	117.49	122.60
14	A	1112	CLA	C4A-NA-C1A	3.53	111.38	106.52
14	L	1502	CLA	C4A-NA-C1A	3.52	111.38	106.52
14	B	1217	CLA	O2D-CGD-CBD	3.52	118.50	111.33
14	A	1124	CLA	C2D-C1D-ND	3.52	112.07	109.41
14	A	1119	CLA	C4A-NA-C1A	3.52	111.37	106.52
14	A	1140	CLA	C4A-NA-C1A	3.52	111.37	106.52
14	A	1139	CLA	C4A-NA-C1A	3.51	111.36	106.52
14	A	1129	CLA	O2D-CGD-CBD	3.51	118.48	111.33
14	B	1221	CLA	C4A-NA-C1A	3.51	111.36	106.52
14	B	1222	CLA	CMB-C2B-C1B	-3.51	123.23	128.62
14	B	1205	CLA	CAA-C2A-C3A	-3.51	104.75	113.04
17	A	4011	BCR	C2-C1-C6	3.50	116.26	110.44
14	B	1232	CLA	C4A-NA-C1A	3.50	111.35	106.52
14	A	1105	CLA	O2A-CGA-CBA	3.50	122.95	111.94
14	A	1128	CLA	C2D-C1D-ND	3.50	112.05	109.41
14	A	1106	CLA	O2A-CGA-CBA	3.50	122.95	111.94
14	B	1201	CLA	O2A-CGA-CBA	3.49	122.92	111.94
14	B	1208	CLA	C4A-NA-C1A	3.49	111.33	106.52
14	B	1229	CLA	O2D-CGD-CBD	3.49	118.44	111.33
17	J	4012	BCR	C29-C30-C25	3.49	116.24	110.44
14	A	1127	CLA	C4A-NA-C1A	3.49	111.33	106.52
14	B	1227	CLA	O2D-CGD-CBD	3.48	118.43	111.33
17	B	4004	BCR	C2-C1-C6	3.48	116.23	110.44
14	B	1206	CLA	C4A-NA-C1A	3.48	111.32	106.52
14	A	1106	CLA	C2D-C1D-ND	3.48	112.04	109.41
14	L	1501	CLA	C4A-NA-C1A	3.47	111.30	106.52
14	A	1136	CLA	C4A-NA-C1A	3.46	111.30	106.52
14	A	1111	CLA	C2B-C3B-CAB	-3.46	120.25	127.33
14	A	1108	CLA	C4A-NA-C1A	3.45	111.28	106.52
17	I	4020	BCR	C33-C5-C4	-3.45	107.00	113.34
14	B	1213	CLA	O2A-CGA-CBA	3.45	122.79	111.94
14	A	1123	CLA	C4A-NA-C1A	3.45	111.28	106.52
17	I	4020	BCR	C38-C26-C27	-3.45	107.01	113.34
14	B	1234	CLA	O2D-CGD-CBD	3.45	118.35	111.33
17	A	4003	BCR	C29-C30-C25	3.45	116.17	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4002	BCR	C38-C26-C27	-3.44	107.02	113.34
14	A	1113	CLA	CMB-C2B-C1B	-3.44	123.33	128.62
14	K	1401	CLA	C4A-NA-C1A	3.44	111.26	106.52
14	B	1224	CLA	C4A-NA-C1A	3.44	111.26	106.52
14	B	1202	CLA	CMB-C2B-C1B	-3.43	123.34	128.62
14	A	1107	CLA	CMB-C2B-C1B	-3.43	123.34	128.62
14	B	1213	CLA	C4A-NA-C1A	3.43	111.25	106.52
14	B	1218	CLA	O2D-CGD-CBD	3.43	118.31	111.33
17	A	4008	BCR	C24-C23-C22	3.42	131.34	126.22
14	A	1135	CLA	C2D-C1D-ND	3.42	112.00	109.41
14	A	1121	CLA	O2D-CGD-CBD	3.42	118.30	111.33
14	A	1115	CLA	C2D-C1D-ND	3.42	111.99	109.41
14	A	1127	CLA	CMB-C2B-C3B	3.42	130.36	124.97
14	J	1302	CLA	O2D-CGD-CBD	3.42	118.29	111.33
14	A	1104	CLA	C4A-NA-C1A	3.41	111.22	106.52
14	A	1126	CLA	C2D-C1D-ND	3.41	111.98	109.41
14	A	1104	CLA	C2A-C3A-C4A	3.41	106.64	101.40
14	A	1121	CLA	C4A-NA-C1A	3.41	111.22	106.52
14	B	1222	CLA	O2A-CGA-CBA	3.40	120.97	110.52
17	L	4019	BCR	C33-C5-C4	-3.40	107.09	113.34
14	A	1127	CLA	C2D-C1D-ND	3.40	111.98	109.41
14	B	1219	CLA	CMB-C2B-C1B	-3.40	123.40	128.62
14	A	1125	CLA	O2A-CGA-CBA	3.40	122.62	111.94
17	F	4016	BCR	C15-C14-C13	3.39	132.18	127.29
14	B	1234	CLA	C4A-NA-C1A	3.39	111.19	106.52
17	B	4009	BCR	C20-C21-C22	3.38	132.17	127.29
14	L	1503	CLA	C4A-NA-C1A	3.38	111.17	106.52
14	B	1210	CLA	O2D-CGD-CBD	3.38	118.21	111.33
14	A	1237	CLA	C2D-C1D-ND	3.37	111.96	109.41
14	B	1202	CLA	O2D-CGD-CBD	3.37	118.20	111.33
17	B	4010	BCR	C33-C5-C4	-3.37	107.16	113.34
14	B	1210	CLA	C2B-C3B-CAB	-3.36	120.45	127.33
17	B	4006	BCR	C33-C5-C4	-3.36	107.17	113.34
14	B	1226	CLA	C4A-NA-C1A	3.36	111.15	106.52
14	A	1109	CLA	O2A-CGA-CBA	3.36	122.50	111.94
17	J	4015	BCR	C33-C5-C4	-3.35	107.19	113.34
14	B	1239	CLA	OBD-CAD-CBD	-3.35	120.89	125.94
14	B	1202	CLA	OBD-CAD-CBD	-3.35	120.88	125.94
14	A	1801	CLA	CBD-CHA-C1A	3.34	133.14	128.77
14	B	1223	CLA	O2D-CGD-CBD	3.34	118.14	111.33
14	B	1207	CLA	C2D-C1D-ND	3.34	111.93	109.41
14	A	1131	CLA	C4A-NA-C1A	3.34	111.13	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1103	CLA	CMB-C2B-C1B	-3.34	123.48	128.62
14	A	1115	CLA	C4A-NA-C1A	3.34	111.12	106.52
17	J	4013	BCR	C2-C1-C6	3.33	115.98	110.44
14	B	1238	CLA	C4A-NA-C1A	3.33	111.12	106.52
14	B	1219	CLA	C2B-C3B-CAB	-3.33	120.51	127.33
14	B	1238	CLA	C4B-C3B-CAB	3.33	133.93	127.18
14	A	1103	CLA	C4A-NA-C1A	3.33	111.11	106.52
14	B	1204	CLA	OBD-CAD-CBD	-3.33	120.91	125.94
14	K	1401	CLA	O2D-CGD-CBD	3.33	118.11	111.33
14	A	1103	CLA	O2D-CGD-CBD	3.33	118.11	111.33
14	B	1023	CLA	C4A-NA-C1A	3.32	111.10	106.52
17	B	4009	BCR	C38-C26-C27	-3.32	107.24	113.34
14	A	1126	CLA	CMB-C2B-C1B	-3.32	123.52	128.62
17	J	4013	BCR	C29-C30-C25	3.32	115.95	110.44
17	I	4018	BCR	C38-C26-C27	-3.32	107.25	113.34
14	A	1120	CLA	O2D-CGD-CBD	3.32	118.08	111.33
14	A	1130	CLA	C1-C2-C3	3.31	132.08	126.19
14	A	1119	CLA	CAA-C2A-C3A	-3.31	105.20	113.04
14	A	1128	CLA	C4A-NA-C1A	3.31	111.09	106.52
17	J	4015	BCR	C38-C26-C27	-3.31	107.26	113.34
14	A	1104	CLA	CMB-C2B-C3B	3.31	130.18	124.97
14	B	1225	CLA	O2A-C1-C2	3.31	115.72	108.55
14	A	1013	CLA	C2D-C1D-ND	3.30	111.90	109.41
14	A	1102	CLA	O2A-CGA-CBA	3.30	122.31	111.94
14	B	1221	CLA	O2D-CGD-CBD	3.30	118.05	111.33
14	L	1501	CLA	O2A-CGA-CBA	3.29	122.30	111.94
14	A	1131	CLA	CMB-C2B-C1B	-3.29	123.56	128.62
14	A	1102	CLA	CMB-C2B-C1B	-3.29	123.56	128.62
17	B	4004	BCR	C24-C23-C22	3.28	131.13	126.22
14	A	1103	CLA	C2B-C3B-CAB	-3.28	120.61	127.33
14	B	1235	CLA	O2A-CGA-CBA	3.28	122.26	111.94
14	A	1124	CLA	CMB-C2B-C3B	3.28	130.13	124.97
14	B	1228	CLA	O2D-CGD-CBD	3.28	118.00	111.33
14	A	1114	CLA	CMB-C2B-C1B	-3.27	123.58	128.62
14	A	1140	CLA	C2D-C1D-ND	3.27	111.88	109.41
17	B	4014	BCR	C38-C26-C27	-3.27	107.33	113.34
14	A	1117	CLA	CMB-C2B-C3B	3.27	130.12	124.97
14	B	1236	CLA	C4A-NA-C1A	3.27	111.02	106.52
14	A	1013	CLA	CMB-C2B-C1B	-3.26	123.61	128.62
14	B	1203	CLA	C2B-C3B-CAB	-3.26	120.66	127.33
14	A	1132	CLA	C4A-NA-C1A	3.26	111.01	106.52
14	A	1013	CLA	C4A-NA-C1A	3.25	111.00	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1203	CLA	C4A-NA-C1A	3.25	111.00	106.52
14	B	1210	CLA	C2D-C1D-ND	3.25	111.86	109.41
14	A	1111	CLA	O2D-CGD-CBD	3.25	117.94	111.33
14	B	1012	CLA	C4A-NA-C1A	3.25	111.00	106.52
14	A	1137	CLA	C4A-NA-C1A	3.24	110.99	106.52
14	A	1101	CLA	O2A-CGA-CBA	3.24	122.14	111.94
14	A	1114	CLA	O2A-CGA-CBA	3.24	122.14	111.94
14	B	1223	CLA	C2D-C1D-ND	3.24	111.86	109.41
14	A	1139	CLA	C2D-C1D-ND	3.24	111.86	109.41
14	A	1129	CLA	O2A-CGA-CBA	3.24	122.12	111.94
14	A	1140	CLA	O2A-C1-C2	3.24	115.56	108.55
14	B	1225	CLA	C4-C3-C5	-3.24	110.47	115.39
14	A	1126	CLA	C4A-NA-C1A	3.24	110.98	106.52
14	A	1133	CLA	C1-C2-C3	3.23	131.93	126.19
14	A	1126	CLA	O2A-CGA-CBA	3.23	122.11	111.94
17	B	4004	BCR	C33-C5-C4	-3.23	107.40	113.34
17	B	4005	BCR	C29-C30-C25	3.23	115.81	110.44
17	L	4022	BCR	C33-C5-C4	-3.23	107.41	113.34
14	A	1108	CLA	CMB-C2B-C1B	-3.23	123.65	128.62
14	B	1231	CLA	O2D-CGD-CBD	3.23	117.91	111.33
14	B	1208	CLA	CAA-C2A-C3A	-3.23	105.41	113.04
14	B	1239	CLA	C2D-C1D-ND	3.23	111.85	109.41
14	A	1237	CLA	C4A-NA-C1A	3.22	110.96	106.52
14	B	1207	CLA	O2A-CGA-CBA	3.22	122.06	111.94
14	A	1129	CLA	C2D-C1D-ND	3.22	111.84	109.41
14	B	1201	CLA	C2D-C1D-ND	3.22	111.84	109.41
14	B	1204	CLA	O2A-CGA-CBA	3.21	122.05	111.94
14	B	1222	CLA	CMB-C2B-C3B	3.21	130.03	124.97
17	A	4007	BCR	C38-C26-C27	-3.21	107.44	113.34
14	A	1104	CLA	C2B-C3B-CAB	-3.21	120.75	127.33
18	A	5001	LHG	O8-C23-C24	3.21	122.04	111.94
17	J	4013	BCR	C7-C8-C9	3.21	131.02	126.22
14	A	1138	CLA	O2A-CGA-CBA	3.21	122.04	111.94
14	B	1223	CLA	CMB-C2B-C3B	3.21	130.03	124.97
14	A	1011	CLA	O2A-CGA-CBA	3.21	122.02	111.94
14	B	1210	CLA	C4A-NA-C1A	3.20	110.93	106.52
17	J	4012	BCR	C2-C1-C6	3.20	115.75	110.44
17	J	4013	BCR	C38-C26-C25	3.20	128.13	124.51
17	F	4016	BCR	C33-C5-C4	-3.20	107.47	113.34
14	A	1130	CLA	O2A-CGA-CBA	3.20	121.99	111.94
14	B	1224	CLA	C2D-C1D-ND	3.19	111.82	109.41
14	A	1132	CLA	C2D-C1D-ND	3.19	111.82	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1222	CLA	C2B-C3B-CAB	-3.18	120.81	127.33
14	B	1210	CLA	CMB-C2B-C3B	3.18	129.98	124.97
17	L	4019	BCR	C38-C26-C27	-3.18	107.50	113.34
14	A	1237	CLA	CAA-C2A-C3A	-3.18	105.53	113.04
14	A	1133	CLA	O2A-CGA-CBA	3.17	121.92	111.94
17	F	4016	BCR	C38-C26-C27	-3.17	107.51	113.34
14	B	1239	CLA	C4B-C3B-CAB	3.17	133.59	127.18
14	B	1207	CLA	C1D-C2D-C3D	-3.17	104.19	106.78
14	A	1113	CLA	C2B-C3B-CAB	-3.16	120.86	127.33
14	B	1223	CLA	O2A-CGA-CBA	3.16	121.88	111.94
17	A	4011	BCR	C29-C30-C25	3.16	115.69	110.44
14	A	1129	CLA	C1D-CHD-C4C	3.16	127.50	122.60
14	A	1140	CLA	CMB-C2B-C1B	-3.16	123.77	128.62
14	A	1135	CLA	CMB-C2B-C1B	-3.15	123.77	128.62
17	A	4003	BCR	C33-C5-C4	-3.15	107.55	113.34
14	A	1111	CLA	O2A-CGA-CBA	3.15	121.86	111.94
14	A	1111	CLA	CMB-C2B-C1B	-3.15	123.77	128.62
14	A	1013	CLA	C2B-C3B-CAB	-3.15	120.88	127.33
17	A	4011	BCR	C33-C5-C4	-3.15	107.56	113.34
14	A	1103	CLA	O2A-CGA-CBA	3.15	121.84	111.94
17	A	4001	BCR	C33-C5-C4	-3.14	107.56	113.34
14	B	1234	CLA	C1-C2-C3	3.14	131.78	126.19
17	A	4002	BCR	C2-C1-C6	3.14	115.66	110.44
17	J	4012	BCR	C23-C24-C25	3.14	136.60	127.32
14	A	1136	CLA	O2A-CGA-CBA	3.14	121.82	111.94
14	A	1135	CLA	C1-C2-C3	3.14	131.76	126.19
14	B	1202	CLA	C4A-NA-C1A	3.14	110.84	106.52
14	B	1219	CLA	C4B-C3B-CAB	3.13	133.51	127.18
17	B	4014	BCR	C2-C1-C6	3.13	115.64	110.44
14	B	1229	CLA	O2A-CGA-CBA	3.13	121.78	111.94
14	B	1224	CLA	CMB-C2B-C1B	-3.13	123.81	128.62
14	B	1210	CLA	O2A-CGA-CBA	3.13	121.77	111.94
17	B	4014	BCR	C29-C30-C25	3.13	115.64	110.44
14	B	1202	CLA	O2A-CGA-CBA	3.13	121.77	111.94
17	B	4004	BCR	C30-C25-C26	-3.12	118.08	122.60
14	B	1219	CLA	C1-C2-C3	3.12	131.73	126.19
17	A	4001	BCR	C29-C30-C25	3.12	115.62	110.44
14	A	1105	CLA	C2D-C1D-ND	3.12	111.77	109.41
14	L	1503	CLA	C2D-C1D-ND	3.12	111.76	109.41
14	B	1204	CLA	O2D-CGD-CBD	3.12	117.68	111.33
14	A	1127	CLA	O2D-CGD-CBD	3.12	117.68	111.33
14	A	1132	CLA	CAA-C2A-C3A	-3.11	105.69	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1011	CLA	C4A-NA-C1A	3.11	110.81	106.52
14	B	1229	CLA	CMB-C2B-C1B	-3.11	123.84	128.62
14	B	1226	CLA	C2D-C1D-ND	3.11	111.76	109.41
14	B	1203	CLA	CMB-C2B-C1B	-3.11	123.84	128.62
14	B	1012	CLA	O2A-CGA-CBA	3.10	121.70	111.94
14	B	1238	CLA	C1-C2-C3	3.10	131.70	126.19
17	B	4004	BCR	C23-C24-C25	3.10	136.49	127.32
14	B	1216	CLA	CMB-C2B-C1B	-3.10	123.85	128.62
14	A	1103	CLA	C2D-C1D-ND	3.10	111.75	109.41
14	A	1114	CLA	O2D-CGD-CBD	3.10	117.64	111.33
14	A	1801	CLA	C2D-C1D-ND	3.10	111.75	109.41
17	B	4017	BCR	C2-C1-C6	3.10	115.59	110.44
17	M	4021	BCR	C2-C1-C6	3.10	115.59	110.44
14	A	1120	CLA	CMB-C2B-C1B	-3.10	123.86	128.62
17	B	4005	BCR	C33-C5-C4	-3.09	107.66	113.34
17	B	4006	BCR	C2-C1-C6	3.09	115.58	110.44
17	L	4019	BCR	C24-C23-C22	3.09	130.84	126.22
14	B	1218	CLA	CMB-C2B-C1B	-3.09	123.86	128.62
14	B	1214	CLA	OBD-CAD-CBD	-3.09	121.27	125.94
14	A	1022	CLA	C4A-NA-C1A	3.09	110.78	106.52
14	B	1021	CLA	C2D-C1D-ND	3.09	111.74	109.41
14	A	1115	CLA	CMB-C2B-C1B	-3.09	123.87	128.62
14	A	1137	CLA	O2D-CGD-CBD	3.09	117.62	111.33
14	B	1202	CLA	C1-C2-C3	3.09	131.67	126.19
17	B	4010	BCR	C2-C1-C6	3.09	115.57	110.44
14	B	1216	CLA	CAA-C2A-C3A	-3.08	105.75	113.04
17	J	4015	BCR	C29-C30-C25	3.08	115.56	110.44
14	A	1119	CLA	C2B-C3B-CAB	-3.08	121.02	127.33
14	L	1502	CLA	CAA-C2A-C3A	-3.08	105.76	113.04
14	A	1130	CLA	O2D-CGD-CBD	3.08	117.60	111.33
14	B	1214	CLA	CMB-C2B-C1B	-3.08	123.89	128.62
14	A	1129	CLA	CAA-C2A-C3A	-3.08	105.77	113.04
14	B	1236	CLA	O2A-CGA-CBA	3.08	121.61	111.94
14	A	1130	CLA	C1D-CHD-C4C	3.07	127.36	122.60
14	A	1104	CLA	C4B-C3B-CAB	3.07	133.40	127.18
19	B	5002	LMG	O8-C28-C29	3.07	121.60	111.94
14	B	1209	CLA	O2D-CGD-CBD	3.07	117.58	111.33
14	B	1023	CLA	C2D-C1D-ND	3.06	111.72	109.41
17	B	4004	BCR	C7-C8-C9	3.06	130.80	126.22
17	B	4017	BCR	C7-C8-C9	3.07	130.80	126.22
14	B	1210	CLA	C4B-C3B-CAB	3.06	133.38	127.18
14	A	1110	CLA	C2D-C1D-ND	3.06	111.72	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1111	CLA	C4B-C3B-CAB	3.06	133.37	127.18
14	A	1134	CLA	CMB-C2B-C1B	-3.06	123.92	128.62
17	A	4001	BCR	C30-C25-C26	-3.06	118.17	122.60
14	A	1124	CLA	C2B-C3B-CAB	-3.05	121.08	127.33
17	L	4022	BCR	C2-C1-C6	3.05	115.52	110.44
14	L	1503	CLA	O2D-CGD-CBD	3.05	117.55	111.33
14	A	1128	CLA	CMB-C2B-C1B	-3.05	123.92	128.62
17	M	4021	BCR	C38-C26-C27	-3.05	107.73	113.34
17	B	4010	BCR	C38-C26-C27	-3.05	107.73	113.34
14	B	1023	CLA	O2A-CGA-CBA	3.05	121.53	111.94
17	F	4016	BCR	C2-C1-C6	3.05	115.51	110.44
14	B	1201	CLA	CMB-C2B-C1B	-3.05	123.93	128.62
14	A	1101	CLA	CMB-C2B-C1B	-3.05	123.94	128.62
14	A	1128	CLA	CAA-C2A-C3A	-3.04	105.84	113.04
14	A	1133	CLA	CMB-C2B-C1B	-3.04	123.94	128.62
14	B	1213	CLA	O2D-CGD-CBD	3.04	117.52	111.33
14	X	1701	CLA	O2D-CGD-CBD	3.04	117.52	111.33
14	B	1212	CLA	CMB-C2B-C1B	-3.04	123.95	128.62
14	B	1205	CLA	O1D-CGD-CBD	-3.04	118.20	124.42
14	B	1209	CLA	C1D-CHD-C4C	3.04	127.31	122.60
14	X	1701	CLA	CMB-C2B-C1B	-3.03	123.95	128.62
14	A	1118	CLA	O2D-CGD-CBD	3.03	117.51	111.33
14	A	1104	CLA	CBD-CHA-C1A	3.03	132.73	128.77
14	A	1113	CLA	C2D-C1D-ND	3.03	111.70	109.41
17	B	4017	BCR	C38-C26-C27	-3.03	107.78	113.34
14	A	1113	CLA	CMB-C2B-C3B	3.02	129.73	124.97
17	A	4002	BCR	C33-C5-C4	-3.02	107.78	113.34
14	B	1226	CLA	O2A-CGA-CBA	3.02	121.45	111.94
14	A	1121	CLA	CMB-C2B-C1B	-3.02	123.97	128.62
14	B	1220	CLA	CMB-C2B-C1B	-3.02	123.97	128.62
14	B	1225	CLA	C4A-NA-C1A	3.02	110.69	106.52
14	B	1228	CLA	C2D-C1D-ND	3.02	111.69	109.41
17	A	4008	BCR	C29-C30-C25	3.02	115.46	110.44
17	L	4019	BCR	C30-C25-C24	3.02	124.05	115.69
14	A	1801	CLA	CMB-C2B-C1B	-3.02	123.98	128.62
14	B	1213	CLA	CMB-C2B-C1B	-3.02	123.98	128.62
14	A	1131	CLA	CMB-C2B-C3B	3.02	129.72	124.97
17	J	4012	BCR	C30-C25-C26	-3.02	118.23	122.60
14	A	1123	CLA	O2A-CGA-CBA	3.02	121.43	111.94
17	B	4009	BCR	C24-C23-C22	3.02	130.73	126.22
14	B	1229	CLA	C2D-C1D-ND	3.01	111.69	109.41
17	A	4011	BCR	C38-C26-C27	-3.01	107.81	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1021	CLA	O2A-CGA-CBA	3.01	121.40	111.94
14	B	1224	CLA	OBD-CAD-CBD	-3.01	121.40	125.94
14	A	1131	CLA	O2D-CGD-CBD	3.01	117.46	111.33
14	A	1013	CLA	C4B-C3B-CAB	3.01	133.26	127.18
14	B	1234	CLA	C2D-C1D-ND	3.01	111.68	109.41
14	B	1221	CLA	O2A-CGA-CBA	3.00	121.38	111.94
17	B	4006	BCR	C28-C27-C26	3.00	118.29	113.74
14	B	1209	CLA	CMB-C2B-C1B	-3.00	124.00	128.62
14	J	1302	CLA	CMB-C2B-C1B	-3.00	124.01	128.62
14	B	1207	CLA	CAA-C2A-C1A	3.00	119.11	111.62
14	B	1012	CLA	CMB-C2B-C1B	-3.00	124.01	128.62
14	B	1224	CLA	O2D-CGD-CBD	3.00	117.44	111.33
17	B	4014	BCR	C8-C9-C10	-3.00	114.36	118.97
14	A	1103	CLA	OBD-CAD-CBD	-3.00	121.41	125.94
14	L	1501	CLA	OBD-CAD-CBD	-2.99	121.42	125.94
14	B	1205	CLA	C4A-NA-C1A	3.00	110.65	106.52
17	B	4010	BCR	C24-C23-C22	3.00	130.70	126.22
17	M	4021	BCR	C29-C30-C25	2.99	115.41	110.44
17	A	4008	BCR	C30-C25-C26	-2.99	118.27	122.60
14	B	1238	CLA	CED-O2D-CGD	2.99	123.13	116.02
14	A	1112	CLA	O2D-CGD-CBD	2.99	117.42	111.33
14	L	1503	CLA	CMB-C2B-C1B	-2.99	124.03	128.62
14	L	1502	CLA	O2D-CGD-CBD	2.99	117.42	111.33
17	F	4016	BCR	C29-C30-C25	2.98	115.40	110.44
14	B	1236	CLA	C2D-C1D-ND	2.98	111.66	109.41
17	B	4006	BCR	C24-C23-C22	2.98	130.67	126.22
14	B	1206	CLA	C2D-C1D-ND	2.98	111.66	109.41
14	B	1219	CLA	O2A-CGA-CBA	2.98	121.31	111.94
14	A	1022	CLA	C1-C2-C3	2.98	131.48	126.19
14	B	1216	CLA	O2A-CGA-CBA	2.98	121.31	111.94
14	A	1124	CLA	O2D-CGD-CBD	2.98	117.39	111.33
14	A	1107	CLA	C2D-C1D-ND	2.98	111.66	109.41
14	A	1130	CLA	C2B-C3B-CAB	-2.97	121.24	127.33
14	B	1225	CLA	CMB-C2B-C1B	-2.98	124.05	128.62
14	B	1225	CLA	C5-C3-C2	2.98	126.81	121.08
14	A	1119	CLA	CED-O2D-CGD	2.97	123.09	116.02
14	A	1132	CLA	C3B-CAB-CBB	-2.97	119.79	125.95
18	A	5003	LHG	C6-C5-C4	-2.97	105.09	111.86
14	B	1235	CLA	OBD-CAD-CBD	-2.97	121.46	125.94
14	B	1217	CLA	CMB-C2B-C1B	-2.97	124.05	128.62
14	B	1239	CLA	O2D-CGD-CBD	2.97	117.38	111.33
14	A	1131	CLA	C2D-C1D-ND	2.97	111.65	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1134	CLA	C1D-CHD-C4C	2.96	127.20	122.60
14	A	1119	CLA	OBD-CAD-CBD	-2.96	121.46	125.94
14	A	1134	CLA	C2D-C1D-ND	2.96	111.65	109.41
14	A	1237	CLA	C1D-C2D-C3D	-2.96	104.36	106.78
14	A	1013	CLA	CMB-C2B-C3B	2.96	129.63	124.97
14	B	1230	CLA	C1-C2-C3	2.96	131.44	126.19
17	I	4018	BCR	C7-C8-C9	2.96	130.64	126.22
14	B	1235	CLA	O2D-CGD-CBD	2.96	117.36	111.33
17	M	4021	BCR	C1-C6-C7	2.96	123.89	115.69
14	B	1229	CLA	OBD-CAD-CBD	-2.96	121.48	125.94
14	A	1116	CLA	CMB-C2B-C1B	-2.96	124.08	128.62
14	A	1139	CLA	O2D-CGD-CBD	2.95	117.34	111.33
14	B	1239	CLA	O2A-CGA-CBA	2.95	121.23	111.94
14	A	1129	CLA	OBD-CAD-CBD	-2.95	121.48	125.94
14	A	1118	CLA	C1D-CHD-C4C	2.95	127.17	122.60
14	A	1121	CLA	C1-C2-C3	2.95	131.43	126.19
14	K	1401	CLA	C2D-C1D-ND	2.95	111.64	109.41
14	A	1138	CLA	CED-O2D-CGD	2.95	123.03	116.02
14	L	1502	CLA	C2D-C1D-ND	2.95	111.64	109.41
17	J	4013	BCR	C30-C25-C24	2.94	123.85	115.69
14	A	1126	CLA	CAA-C2A-C3A	-2.94	106.08	113.04
17	A	4007	BCR	C29-C30-C25	2.94	115.33	110.44
17	B	4004	BCR	C29-C30-C25	2.94	115.33	110.44
17	J	4013	BCR	C33-C5-C4	-2.94	107.94	113.34
14	B	1228	CLA	O2A-CGA-CBA	2.94	121.18	111.94
14	A	1119	CLA	C4B-C3B-CAB	2.94	133.12	127.18
14	B	1225	CLA	C2D-C1D-ND	2.94	111.63	109.41
14	B	1236	CLA	CMB-C2B-C1B	-2.93	124.11	128.62
14	M	1601	CLA	C1D-CHD-C4C	2.93	127.15	122.60
14	A	1103	CLA	CMB-C2B-C3B	2.93	129.59	124.97
14	A	1135	CLA	O2D-CGD-CBD	2.93	117.31	111.33
14	A	1126	CLA	C2B-C3B-CAB	-2.93	121.32	127.33
17	J	4015	BCR	C1-C6-C5	-2.93	118.35	122.60
14	B	1220	CLA	O2D-CGD-CBD	2.93	117.31	111.33
14	A	1122	CLA	O2A-CGA-CBA	2.93	121.17	111.94
14	B	1222	CLA	C1D-CHD-C4C	2.93	127.15	122.60
17	A	4011	BCR	C16-C17-C18	2.93	131.51	127.29
18	B	5004	LHG	O7-C7-C8	2.93	117.98	111.56
14	B	1233	CLA	C2D-C1D-ND	2.93	111.62	109.41
14	L	1501	CLA	C1D-C2D-C3D	-2.93	104.39	106.78
14	A	1022	CLA	CMB-C2B-C1B	-2.93	124.12	128.62
14	B	1206	CLA	O2A-CGA-CBA	2.93	121.15	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1220	CLA	OBD-CAD-CBD	-2.93	121.52	125.94
14	B	1230	CLA	O2A-CGA-CBA	2.93	121.14	111.94
14	B	1239	CLA	CMB-C2B-C1B	-2.92	124.12	128.62
14	B	1215	CLA	O2D-CGD-CBD	2.92	117.29	111.33
14	A	1112	CLA	OBD-CAD-CBD	-2.92	121.53	125.94
14	B	1202	CLA	CMB-C2B-C3B	2.92	129.57	124.97
14	B	1232	CLA	C2D-C1D-ND	2.92	111.61	109.41
14	B	1222	CLA	C2A-C3A-C4A	2.92	105.89	101.40
14	A	1118	CLA	C1-C2-C3	2.91	131.37	126.19
14	A	1138	CLA	CMB-C2B-C1B	-2.91	124.14	128.62
14	A	1022	CLA	O2D-CGD-CBD	2.91	117.26	111.33
14	B	1217	CLA	C1D-CHD-C4C	2.91	127.11	122.60
14	A	1108	CLA	C2D-C1D-ND	2.91	111.61	109.41
14	L	1503	CLA	OBD-CAD-CBD	-2.91	121.55	125.94
14	A	1115	CLA	O2A-CGA-CBA	2.91	121.09	111.94
14	J	1302	CLA	C1D-CHD-C4C	2.91	127.11	122.60
17	A	4003	BCR	C2-C1-C6	2.91	115.27	110.44
17	B	4014	BCR	C12-C13-C14	-2.91	114.50	118.97
14	A	1112	CLA	CMB-C2B-C1B	-2.91	124.15	128.62
17	A	4003	BCR	C7-C8-C9	2.90	130.56	126.22
14	A	1237	CLA	O2A-CGA-O1A	-2.90	115.50	123.43
14	B	1203	CLA	CMB-C2B-C3B	2.90	129.54	124.97
14	L	1502	CLA	O2A-CGA-CBA	2.90	121.08	111.94
14	B	1230	CLA	C2D-C1D-ND	2.90	111.60	109.41
17	F	4016	BCR	C24-C23-C22	2.90	130.56	126.22
14	K	1401	CLA	CMB-C2B-C1B	-2.90	124.16	128.62
14	A	1122	CLA	CMB-C2B-C1B	-2.90	124.17	128.62
17	A	4007	BCR	C33-C5-C4	-2.90	108.02	113.34
14	B	1211	CLA	CMB-C2B-C1B	-2.90	124.16	128.62
14	B	1215	CLA	C2D-C1D-ND	2.90	111.60	109.41
17	I	4020	BCR	C3-C4-C5	2.89	118.13	113.74
14	J	1303	CLA	C1D-CHD-C4C	2.89	127.09	122.60
14	L	1503	CLA	O2A-CGA-CBA	2.89	121.04	111.94
17	A	4007	BCR	C30-C25-C24	2.89	123.70	115.69
14	B	1213	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
14	A	1116	CLA	OBD-CAD-CBD	-2.89	121.57	125.94
17	A	4007	BCR	C2-C1-C6	2.89	115.24	110.44
17	B	4017	BCR	C33-C5-C4	-2.89	108.03	113.34
14	A	1126	CLA	CMB-C2B-C3B	2.88	129.51	124.97
14	B	1238	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
14	B	1205	CLA	CMB-C2B-C1B	-2.88	124.19	128.62
14	A	1237	CLA	CMB-C2B-C1B	-2.88	124.19	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1221	CLA	OBD-CAD-CBD	-2.88	121.59	125.94
14	A	1132	CLA	C1D-C2D-C3D	-2.88	104.43	106.78
14	B	1228	CLA	CMB-C2B-C1B	-2.88	124.19	128.62
14	A	1126	CLA	OBD-CAD-CBD	-2.88	121.59	125.94
14	B	1208	CLA	C2D-C1D-ND	2.87	111.58	109.41
18	A	5001	LHG	O7-C7-C8	2.87	117.86	111.56
14	A	1011	CLA	C4D-C3D-CAD	-2.87	104.52	108.05
14	B	1219	CLA	CMB-C2B-C3B	2.87	129.49	124.97
14	A	1013	CLA	CED-O2D-CGD	2.87	122.85	116.02
14	B	1227	CLA	C1D-CHD-C4C	2.87	127.05	122.60
14	B	1216	CLA	C2D-C1D-ND	2.87	111.58	109.41
17	B	4005	BCR	C1-C6-C5	-2.87	118.45	122.60
17	A	4001	BCR	C24-C23-C22	2.87	130.51	126.22
17	J	4012	BCR	C33-C5-C4	-2.87	108.07	113.34
14	B	1202	CLA	C2B-C3B-CAB	-2.87	121.45	127.33
14	F	1301	CLA	C2D-C1D-ND	2.87	111.58	109.41
14	X	1701	CLA	C1D-CHD-C4C	2.86	127.04	122.60
17	B	4004	BCR	C1-C6-C5	-2.86	118.46	122.60
14	B	1012	CLA	C2D-C1D-ND	2.86	111.57	109.41
14	B	1211	CLA	O2A-CGA-CBA	2.86	120.93	111.94
17	B	4005	BCR	C1-C6-C7	2.86	123.60	115.69
14	B	1222	CLA	C4B-C3B-CAB	2.85	132.96	127.18
14	B	1023	CLA	OBD-CAD-CBD	-2.85	121.63	125.94
14	B	1230	CLA	CMB-C2B-C1B	-2.85	124.24	128.62
14	M	1601	CLA	CMB-C2B-C1B	-2.85	124.24	128.62
14	B	1205	CLA	C2D-C1D-ND	2.85	111.56	109.41
14	A	1110	CLA	O2D-CGD-CBD	2.85	117.13	111.33
14	B	1221	CLA	CMB-C2B-C1B	-2.85	124.24	128.62
14	A	1133	CLA	C2D-C1D-ND	2.84	111.56	109.41
14	A	1108	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
14	A	1115	CLA	O2D-CGD-CBD	2.84	117.12	111.33
14	A	1134	CLA	O2D-CGD-CBD	2.84	117.12	111.33
17	A	4003	BCR	C40-C30-C25	2.84	115.04	110.33
14	A	1118	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
14	B	1231	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
14	B	1215	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
14	A	1124	CLA	O2A-CGA-CBA	2.84	120.87	111.94
17	A	4001	BCR	C2-C1-C6	2.84	115.16	110.44
14	A	1105	CLA	O2D-CGD-CBD	2.84	117.11	111.33
14	A	1114	CLA	CED-O2D-CGD	2.84	122.77	116.02
14	B	1201	CLA	C1D-C2D-C3D	-2.83	104.47	106.78
14	A	1103	CLA	C4B-C3B-CAB	2.83	132.91	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1228	CLA	C1D-C2D-C3D	-2.83	104.47	106.78
17	B	4005	BCR	C2-C1-C6	2.83	115.14	110.44
14	B	1232	CLA	OBD-CAD-CBD	-2.83	121.67	125.94
14	A	1130	CLA	CMB-C2B-C1B	-2.83	124.27	128.62
14	A	1107	CLA	C1D-CHD-C4C	2.83	126.98	122.60
17	A	4007	BCR	C30-C25-C26	-2.83	118.50	122.60
14	A	1402	CLA	C2D-C1D-ND	2.83	111.55	109.41
14	B	1021	CLA	OBD-CAD-CBD	-2.83	121.67	125.94
14	A	1118	CLA	C2D-C1D-ND	2.83	111.55	109.41
14	B	1211	CLA	OBD-CAD-CBD	-2.83	121.67	125.94
14	B	1021	CLA	CAA-C2A-C3A	-2.83	106.36	113.04
17	M	4021	BCR	C33-C5-C4	-2.82	108.15	113.34
17	I	4020	BCR	C7-C8-C9	2.82	130.44	126.22
14	A	1129	CLA	C2C-C1C-NC	-2.82	107.88	110.17
14	L	1503	CLA	C1D-CHD-C4C	2.82	126.97	122.60
14	A	1124	CLA	C1D-C2D-C3D	-2.82	104.48	106.78
14	M	1601	CLA	CED-O2D-CGD	2.82	122.73	116.02
14	A	1131	CLA	O2A-CGA-CBA	2.82	120.80	111.94
14	B	1223	CLA	C2B-C3B-CAB	-2.81	121.57	127.33
14	A	1013	CLA	O2A-CGA-O1A	-2.81	115.76	123.43
17	I	4018	BCR	C33-C5-C4	-2.81	108.18	113.34
14	A	1116	CLA	C2D-C1D-ND	2.81	111.53	109.41
14	B	1222	CLA	CBD-CHA-C1A	2.80	132.43	128.77
14	A	1011	CLA	CMB-C2B-C1B	-2.80	124.31	128.62
14	A	1133	CLA	O2D-CGD-CBD	2.80	117.04	111.33
14	A	1104	CLA	CED-O2D-CGD	2.80	122.69	116.02
18	A	5003	LHG	O7-C7-C8	2.80	117.69	111.56
14	A	1136	CLA	OBD-CAD-CBD	-2.80	121.71	125.94
14	F	1301	CLA	CMB-C2B-C1B	-2.80	124.32	128.62
14	B	1210	CLA	C1D-C2D-C3D	-2.80	104.50	106.78
14	M	1601	CLA	C2D-C1D-ND	2.80	111.52	109.41
14	A	1103	CLA	C2A-C3A-C4A	2.80	105.70	101.40
17	B	4009	BCR	C29-C30-C25	2.79	115.08	110.44
14	A	1131	CLA	C2B-C3B-CAB	-2.79	121.61	127.33
17	L	4022	BCR	C38-C26-C27	-2.79	108.21	113.34
14	B	1235	CLA	CED-O2D-CGD	2.79	122.66	116.02
14	A	1132	CLA	OBD-CAD-CBD	-2.79	121.72	125.94
14	B	1231	CLA	C2A-C3A-C4A	2.79	105.69	101.40
17	A	4011	BCR	C30-C25-C24	2.79	123.42	115.69
14	L	1502	CLA	OBD-CAD-CBD	-2.79	121.73	125.94
14	B	1238	CLA	C2D-C1D-ND	2.79	111.52	109.41
14	A	1119	CLA	C1-C2-C3	2.79	131.14	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	1501	CLA	C2D-C1D-ND	2.78	111.51	109.41
14	A	1113	CLA	C4B-C3B-CAB	2.78	132.82	127.18
14	J	1303	CLA	CMB-C2B-C1B	-2.78	124.34	128.62
14	B	1219	CLA	C2D-C1D-ND	2.78	111.51	109.41
14	A	1130	CLA	CAA-C2A-C3A	-2.78	106.46	113.04
17	B	4014	BCR	C15-C14-C13	2.78	131.30	127.29
14	B	1012	CLA	C1D-C2D-C3D	-2.78	104.51	106.78
14	A	1104	CLA	CBA-CAA-C2A	2.78	122.26	114.01
14	B	1236	CLA	OBD-CAD-CBD	-2.78	121.74	125.94
14	A	1011	CLA	C2A-C3A-C4A	2.78	105.67	101.40
17	M	4021	BCR	C1-C6-C5	-2.78	118.58	122.60
14	A	1120	CLA	C1D-CHD-C4C	2.78	126.90	122.60
14	A	1109	CLA	CMB-C2B-C1B	-2.78	124.35	128.62
14	A	1110	CLA	CMB-C2B-C1B	-2.77	124.35	128.62
17	J	4012	BCR	C36-C18-C19	2.78	122.58	118.09
14	A	1113	CLA	C1D-CHD-C4C	2.77	126.90	122.60
14	A	1402	CLA	CMB-C2B-C1B	-2.77	124.36	128.62
14	F	1301	CLA	C1D-CHD-C4C	2.77	126.90	122.60
14	A	1124	CLA	C4B-C3B-CAB	2.77	132.79	127.18
14	B	1021	CLA	CBD-CHA-C1A	2.77	132.39	128.77
14	A	1126	CLA	C4B-C3B-CAB	2.77	132.78	127.18
17	J	4013	BCR	C38-C26-C27	-2.77	108.25	113.34
14	A	1130	CLA	CMB-C2B-C3B	2.77	129.33	124.97
14	A	1125	CLA	CMB-C2B-C1B	-2.77	124.37	128.62
17	B	4006	BCR	C1-C6-C5	-2.77	118.59	122.60
14	B	1214	CLA	C2D-C1D-ND	2.77	111.50	109.41
14	A	1122	CLA	CAA-C2A-C3A	-2.76	106.50	113.04
14	A	1105	CLA	CMB-C2B-C1B	-2.76	124.37	128.62
14	A	1103	CLA	C1D-CHD-C4C	2.76	126.89	122.60
14	B	1206	CLA	OBD-CAD-CBD	-2.76	121.77	125.94
14	A	1114	CLA	C2D-C1D-ND	2.76	111.50	109.41
17	B	4006	BCR	C30-C25-C26	-2.76	118.60	122.60
14	B	1023	CLA	CED-O2D-CGD	2.76	122.58	116.02
14	B	1226	CLA	C1-C2-C3	2.76	131.09	126.19
14	B	1218	CLA	C1D-CHD-C4C	2.75	126.87	122.60
14	B	1208	CLA	CED-O2D-CGD	2.75	122.57	116.02
17	L	4019	BCR	C2-C1-C6	2.75	115.02	110.44
14	B	1207	CLA	C2A-C1A-CHA	2.75	128.60	123.83
14	A	1013	CLA	CAA-C2A-C3A	-2.75	106.54	113.04
14	A	1110	CLA	C1-C2-C3	2.75	131.07	126.19
14	A	1126	CLA	C1D-C2D-C3D	-2.75	104.54	106.78
14	B	1220	CLA	C2D-C1D-ND	2.74	111.48	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1106	CLA	OBD-CAD-CBD	-2.74	121.80	125.94
14	A	1135	CLA	CMB-C2B-C3B	2.74	129.29	124.97
14	B	1021	CLA	C7-C6-C5	-2.74	104.94	113.01
14	A	1801	CLA	C1D-CHD-C4C	2.74	126.85	122.60
17	B	4005	BCR	C23-C24-C25	2.74	135.40	127.32
14	A	1119	CLA	C1D-CHD-C4C	2.74	126.85	122.60
14	B	1203	CLA	C4B-C3B-CAB	2.74	132.72	127.18
14	X	1701	CLA	C2D-C1D-ND	2.74	111.48	109.41
14	A	1132	CLA	O2A-CGA-CBA	2.73	120.54	111.94
14	A	1111	CLA	C2D-C1D-ND	2.73	111.47	109.41
14	A	1120	CLA	C2D-C1D-ND	2.73	111.47	109.41
14	B	1229	CLA	C1D-CHD-C4C	2.73	126.83	122.60
14	A	1131	CLA	OBD-CAD-CBD	-2.73	121.82	125.94
14	B	1221	CLA	CED-O2D-CGD	2.73	122.51	116.02
17	J	4012	BCR	C1-C6-C7	2.72	123.24	115.69
14	B	1230	CLA	C1D-C2D-C3D	-2.72	104.56	106.78
17	B	4005	BCR	C20-C21-C22	2.72	131.22	127.29
14	M	1601	CLA	CBD-CHA-C1A	2.72	132.33	128.77
14	A	1011	CLA	CAA-C2A-C3A	-2.72	106.61	113.04
14	J	1302	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
14	A	1136	CLA	CMB-C2B-C1B	-2.72	124.44	128.62
14	B	1233	CLA	O2D-CGD-CBD	2.72	116.87	111.33
14	B	1213	CLA	C2D-C1D-ND	2.72	111.46	109.41
14	B	1208	CLA	CMB-C2B-C1B	-2.72	124.44	128.62
14	A	1111	CLA	C1D-C2D-C3D	-2.72	104.56	106.78
14	B	1238	CLA	CMB-C2B-C1B	-2.72	124.44	128.62
14	A	1125	CLA	C2D-C1D-ND	2.72	111.46	109.41
17	B	4017	BCR	C29-C30-C25	2.72	114.95	110.44
14	B	1210	CLA	C1-C2-C3	2.71	131.01	126.19
14	B	1217	CLA	CED-O2D-CGD	2.72	122.48	116.02
14	B	1233	CLA	C1D-CHD-C4C	2.71	126.81	122.60
17	A	4002	BCR	C29-C30-C25	2.71	114.95	110.44
14	A	1101	CLA	C2D-C1D-ND	2.71	111.46	109.41
14	B	1203	CLA	O2A-CGA-CBA	2.71	120.47	111.94
14	A	1107	CLA	O2D-CGD-CBD	2.71	116.85	111.33
14	B	1211	CLA	CAA-C2A-C3A	-2.71	106.63	113.04
14	B	1206	CLA	O2D-CGD-CBD	2.71	116.85	111.33
17	J	4012	BCR	C8-C7-C6	2.71	135.31	127.32
14	A	1135	CLA	O2A-CGA-O1A	-2.71	116.04	123.43
14	L	1501	CLA	CMB-C2B-C1B	-2.71	124.46	128.62
17	B	4009	BCR	C40-C30-C25	2.71	114.81	110.33
17	A	4001	BCR	C1-C6-C5	-2.70	118.69	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1128	CLA	OBD-CAD-CBD	-2.70	121.86	125.94
14	A	1106	CLA	C1D-C2D-C3D	-2.70	104.57	106.78
17	A	4002	BCR	C30-C25-C26	-2.70	118.69	122.60
14	A	1104	CLA	C1-C2-C3	2.70	130.99	126.19
14	A	1130	CLA	C2D-C1D-ND	2.70	111.45	109.41
14	B	1023	CLA	CMB-C2B-C1B	-2.70	124.47	128.62
14	B	1230	CLA	CED-O2D-CGD	2.70	122.44	116.02
17	I	4020	BCR	C32-C1-C6	2.70	114.80	110.33
14	A	1120	CLA	OBD-CAD-CBD	-2.70	121.87	125.94
14	A	1139	CLA	CMB-C2B-C1B	-2.69	124.48	128.62
14	A	1013	CLA	O2A-C1-C2	-2.69	102.71	108.55
14	A	1107	CLA	C2A-C1A-CHA	2.69	128.50	123.83
17	B	4010	BCR	C30-C25-C24	2.69	123.15	115.69
14	B	1213	CLA	C1-C2-C3	2.69	130.97	126.19
17	A	4001	BCR	C23-C24-C25	2.69	135.26	127.32
17	A	4011	BCR	C32-C1-C6	2.69	114.78	110.33
14	A	1111	CLA	OBD-CAD-CBD	-2.69	121.88	125.94
14	B	1210	CLA	O1D-CGD-CBD	-2.69	118.91	124.42
14	B	1231	CLA	CED-O2D-CGD	2.69	122.41	116.02
14	B	1233	CLA	CMB-C2B-C1B	-2.69	124.49	128.62
14	A	1101	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
14	B	1222	CLA	CAA-C2A-C3A	-2.68	106.70	113.04
19	B	5002	LMG	C7-O1-C1	2.68	119.15	113.81
14	B	1219	CLA	C1D-CHD-C4C	2.68	126.76	122.60
14	B	1214	CLA	C1D-CHD-C4C	2.68	126.75	122.60
14	F	1301	CLA	O2D-CGD-CBD	2.68	116.78	111.33
14	A	1118	CLA	CMB-C2B-C1B	-2.68	124.50	128.62
14	B	1234	CLA	O2A-CGA-CBA	2.68	120.36	111.94
14	B	1219	CLA	CED-O2D-CGD	2.67	122.38	116.02
14	A	1111	CLA	CMB-C2B-C3B	2.67	129.18	124.97
14	B	1238	CLA	C3B-CAB-CBB	-2.67	120.41	125.95
14	A	1102	CLA	C2D-C1D-ND	2.67	111.43	109.41
14	B	1214	CLA	CAA-C2A-C3A	-2.67	106.72	113.04
14	A	1123	CLA	CMB-C2B-C1B	-2.67	124.51	128.62
14	B	1231	CLA	C2D-C1D-ND	2.67	111.43	109.41
14	B	1204	CLA	C1D-CHD-C4C	2.67	126.74	122.60
17	A	4003	BCR	C1-C6-C5	-2.67	118.74	122.60
17	I	4020	BCR	C30-C25-C26	-2.67	118.74	122.60
14	B	1202	CLA	C4B-C3B-CAB	2.67	132.58	127.18
14	A	1125	CLA	C1D-C2D-C3D	-2.67	104.60	106.78
14	A	1117	CLA	C4-C3-C5	-2.66	111.34	115.39
17	I	4018	BCR	C36-C18-C19	2.66	122.40	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1013	CLA	C1D-C2D-C3D	-2.66	104.61	106.78
17	J	4015	BCR	C30-C25-C26	-2.66	118.75	122.60
14	B	1218	CLA	CED-O2D-CGD	2.66	122.35	116.02
17	A	4008	BCR	C2-C1-C6	2.66	114.86	110.44
14	A	1111	CLA	C1D-CHD-C4C	2.66	126.72	122.60
14	A	1109	CLA	CBD-CHA-C1A	2.66	132.25	128.77
14	J	1302	CLA	CED-O2D-CGD	2.66	122.34	116.02
14	A	1137	CLA	CMB-C2B-C1B	-2.66	124.54	128.62
14	B	1207	CLA	O2D-CGD-CBD	2.66	116.74	111.33
14	A	1117	CLA	CED-O2D-CGD	2.65	122.33	116.02
14	A	1133	CLA	C5-C6-C7	-2.65	108.27	113.25
14	A	1122	CLA	O2D-CGD-CBD	2.65	116.73	111.33
14	A	1237	CLA	OBD-CAD-CBD	-2.65	121.94	125.94
14	A	1112	CLA	C2D-C1D-ND	2.65	111.41	109.41
14	B	1222	CLA	C2D-C1D-ND	2.65	111.41	109.41
14	A	1114	CLA	OBD-CAD-CBD	-2.64	121.95	125.94
14	X	1701	CLA	OBD-CAD-CBD	-2.65	121.95	125.94
14	B	1238	CLA	C1D-C2D-C3D	-2.64	104.62	106.78
17	L	4019	BCR	C30-C25-C26	-2.64	118.78	122.60
14	B	1223	CLA	C1D-C2D-C3D	-2.64	104.62	106.78
14	B	1216	CLA	O2D-CGD-CBD	2.64	116.71	111.33
14	A	1117	CLA	C1D-CHD-C4C	2.64	126.69	122.60
14	B	1205	CLA	OBD-CAD-CBD	-2.64	121.96	125.94
14	B	1215	CLA	C1D-CHD-C4C	2.64	126.69	122.60
14	B	1216	CLA	C1D-CHD-C4C	2.64	126.69	122.60
14	A	1128	CLA	O2A-CGA-CBA	2.64	120.23	111.94
14	B	1232	CLA	C1D-CHD-C4C	2.63	126.68	122.60
14	L	1502	CLA	CMB-C2B-C1B	-2.63	124.57	128.62
14	B	1208	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
14	B	1232	CLA	CED-O2D-CGD	2.63	122.28	116.02
14	B	1021	CLA	CED-O2D-CGD	2.63	122.28	116.02
14	A	1138	CLA	C2D-C1D-ND	2.63	111.39	109.41
14	A	1801	CLA	O1D-CGD-CBD	-2.63	119.04	124.42
14	A	1137	CLA	O2A-CGA-O1A	-2.62	116.26	123.43
14	B	1230	CLA	O1D-CGD-CBD	-2.62	119.04	124.42
14	A	1102	CLA	CMB-C2B-C3B	2.63	129.10	124.97
14	B	1218	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
14	A	1129	CLA	C1D-C2D-C3D	-2.62	104.64	106.78
14	K	1401	CLA	C1D-CHD-C4C	2.62	126.67	122.60
17	B	4017	BCR	C8-C9-C10	-2.62	114.94	118.97
14	A	1130	CLA	CED-O2D-CGD	2.62	122.25	116.02
14	A	1123	CLA	OBD-CAD-CBD	-2.62	121.98	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1223	CLA	C4B-C3B-CAB	2.62	132.48	127.18
14	A	1402	CLA	C1D-CHD-C4C	2.62	126.66	122.60
14	L	1503	CLA	C1D-C2D-C3D	-2.62	104.64	106.78
14	B	1221	CLA	C1D-CHD-C4C	2.62	126.66	122.60
17	L	4019	BCR	C40-C30-C25	2.62	114.66	110.33
14	A	1102	CLA	O1D-CGD-CBD	-2.61	119.06	124.42
14	B	1239	CLA	CMB-C2B-C3B	2.61	129.08	124.97
14	A	1103	CLA	CED-O2D-CGD	2.61	122.23	116.02
17	A	4008	BCR	C11-C10-C9	2.61	131.05	127.29
14	B	1219	CLA	O2D-CGD-CBD	2.61	116.64	111.33
14	B	1231	CLA	C1D-CHD-C4C	2.61	126.64	122.60
14	B	1203	CLA	C2D-C1D-ND	2.60	111.38	109.41
14	A	1140	CLA	CED-O2D-CGD	2.60	122.21	116.02
14	B	1235	CLA	CMB-C2B-C1B	-2.60	124.61	128.62
14	A	1109	CLA	CED-O2D-CGD	2.60	122.21	116.02
14	B	1220	CLA	C1D-CHD-C4C	2.60	126.64	122.60
14	B	1218	CLA	C2D-C1D-ND	2.60	111.38	109.41
14	A	1116	CLA	O2D-CGD-CBD	2.60	116.63	111.33
17	B	4014	BCR	C32-C1-C6	2.60	114.63	110.33
14	B	1234	CLA	CMB-C2B-C1B	-2.60	124.62	128.62
14	A	1135	CLA	C2B-C3B-CAB	-2.60	122.01	127.33
14	A	1125	CLA	C1-C2-C3	2.60	130.80	126.19
14	A	1101	CLA	C1D-CHD-C4C	2.60	126.63	122.60
14	B	1227	CLA	CMB-C2B-C1B	-2.59	124.63	128.62
14	A	1123	CLA	C2D-C1D-ND	2.59	111.37	109.41
14	A	1116	CLA	CED-O2D-CGD	2.59	122.19	116.02
17	B	4010	BCR	C36-C18-C19	2.59	122.28	118.09
17	L	4022	BCR	C8-C7-C6	2.59	134.97	127.32
14	A	1130	CLA	C1D-C2D-C3D	-2.59	104.66	106.78
14	A	1123	CLA	O1D-CGD-CBD	-2.59	119.11	124.42
14	A	1112	CLA	CED-O2D-CGD	2.59	122.18	116.02
14	A	1801	CLA	C2C-C1C-NC	-2.59	108.07	110.17
14	A	1121	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
14	A	1111	CLA	O1D-CGD-CBD	-2.59	119.11	124.42
14	A	1129	CLA	CMB-C2B-C1B	-2.59	124.64	128.62
14	B	1216	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
17	F	4016	BCR	C1-C6-C5	-2.59	118.85	122.60
14	A	1124	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
14	M	1601	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
17	A	4003	BCR	C30-C25-C26	-2.59	118.86	122.60
14	A	1117	CLA	C2B-C3B-CAB	-2.58	122.04	127.33
17	B	4010	BCR	C30-C25-C26	-2.58	118.86	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	I	4020	BCR	C37-C22-C23	2.58	122.27	118.09
14	B	1211	CLA	O1D-CGD-CBD	-2.58	119.13	124.42
14	B	1227	CLA	O1D-CGD-CBD	-2.58	119.13	124.42
17	A	4011	BCR	C1-C6-C7	2.58	122.83	115.69
14	A	1108	CLA	O2D-CGD-CBD	2.58	116.58	111.33
14	A	1137	CLA	OBD-CAD-CBD	-2.57	122.05	125.94
14	B	1224	CLA	C1D-CHD-C4C	2.57	126.59	122.60
17	L	4022	BCR	C29-C30-C25	2.57	114.72	110.44
14	B	1012	CLA	C1D-CHD-C4C	2.57	126.59	122.60
17	L	4022	BCR	C30-C25-C26	-2.57	118.88	122.60
14	B	1238	CLA	O2A-CGA-CBA	2.57	120.02	111.94
17	B	4014	BCR	C30-C25-C26	-2.57	118.88	122.60
14	A	1114	CLA	C1D-CHD-C4C	2.56	126.58	122.60
14	A	1131	CLA	C1D-C2D-C3D	-2.56	104.69	106.78
14	A	1122	CLA	OBD-CAD-CBD	-2.56	122.07	125.94
14	B	1202	CLA	C2A-C3A-C4A	2.56	105.34	101.40
14	A	1127	CLA	OBD-CAD-CBD	-2.56	122.07	125.94
17	B	4010	BCR	C16-C17-C18	2.56	130.98	127.29
17	A	4008	BCR	C23-C24-C25	2.56	134.87	127.32
14	A	1133	CLA	CED-O2D-CGD	2.56	122.10	116.02
14	A	1130	CLA	C2A-C3A-C4A	2.56	105.33	101.40
14	A	1127	CLA	C1D-CHD-C4C	2.56	126.56	122.60
17	F	4016	BCR	C30-C25-C26	-2.55	118.90	122.60
17	A	4008	BCR	C1-C6-C7	2.55	122.76	115.69
14	B	1212	CLA	C1D-C2D-C3D	-2.55	104.70	106.78
17	A	4001	BCR	C8-C7-C6	2.55	134.85	127.32
14	A	1106	CLA	CMB-C2B-C1B	-2.55	124.70	128.62
14	A	1106	CLA	O1D-CGD-CBD	-2.55	119.19	124.42
14	B	1203	CLA	C1-C2-C3	2.55	130.72	126.19
14	A	1108	CLA	CED-O2D-CGD	2.55	122.08	116.02
14	A	1140	CLA	OBD-CAD-CBD	-2.55	122.09	125.94
14	B	1214	CLA	CED-O2D-CGD	2.55	122.08	116.02
14	B	1234	CLA	C1D-CHD-C4C	2.55	126.55	122.60
14	A	1117	CLA	OBD-CAD-CBD	-2.55	122.10	125.94
14	B	1205	CLA	O2A-CGA-O1A	-2.55	116.48	123.43
14	B	1202	CLA	C1D-C2D-C3D	-2.54	104.70	106.78
17	B	4010	BCR	C29-C30-C25	2.55	114.67	110.44
14	B	1228	CLA	OBD-CAD-CBD	-2.54	122.10	125.94
17	A	4003	BCR	C1-C6-C7	2.54	122.73	115.69
14	B	1012	CLA	C2A-C1A-CHA	2.54	128.24	123.83
14	A	1129	CLA	O1D-CGD-CBD	-2.54	119.21	124.42
17	L	4019	BCR	C8-C7-C6	2.54	134.83	127.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1236	CLA	O2D-CGD-CBD	2.54	116.51	111.33
14	B	1231	CLA	CMB-C2B-C1B	-2.54	124.71	128.62
17	A	4011	BCR	C15-C14-C13	2.54	130.95	127.29
17	A	4008	BCR	C33-C5-C4	-2.54	108.68	113.34
14	A	1104	CLA	C1D-CHD-C4C	2.54	126.53	122.60
14	B	1231	CLA	CAA-C2A-C3A	-2.53	107.05	113.04
14	B	1212	CLA	CBD-CHA-C1A	2.53	132.08	128.77
14	B	1212	CLA	O1D-CGD-CBD	-2.53	119.23	124.42
14	A	1116	CLA	C1D-CHD-C4C	2.53	126.53	122.60
14	A	1117	CLA	C2D-C1D-ND	2.53	111.32	109.41
17	I	4018	BCR	C23-C24-C25	2.53	134.79	127.32
14	A	1133	CLA	C1D-CHD-C4C	2.53	126.52	122.60
17	I	4020	BCR	C30-C25-C24	2.53	122.69	115.69
17	A	4002	BCR	C30-C25-C24	2.53	122.69	115.69
17	B	4014	BCR	C34-C9-C8	2.53	122.18	118.09
14	B	1217	CLA	C2D-C1D-ND	2.53	111.32	109.41
14	A	1120	CLA	C2A-C3A-C4A	2.53	105.28	101.40
17	J	4012	BCR	C1-C6-C5	-2.53	118.94	122.60
14	B	1227	CLA	C1D-C2D-C3D	-2.52	104.72	106.78
17	A	4003	BCR	C30-C25-C24	2.52	122.68	115.69
14	J	1303	CLA	C2D-C1D-ND	2.52	111.31	109.41
14	K	1401	CLA	C1D-C2D-C3D	-2.52	104.72	106.78
14	A	1013	CLA	CBD-CHA-C1A	2.52	132.06	128.77
14	A	1110	CLA	C1D-CHD-C4C	2.52	126.50	122.60
14	L	1502	CLA	C1D-C2D-C3D	-2.52	104.73	106.78
17	J	4013	BCR	C30-C25-C26	-2.52	118.96	122.60
14	A	1115	CLA	CED-O2D-CGD	2.51	122.00	116.02
14	B	1021	CLA	C1-C2-C3	2.51	130.66	126.19
14	B	1206	CLA	CED-O2D-CGD	2.51	122.00	116.02
14	B	1204	CLA	C1D-C2D-C3D	-2.51	104.73	106.78
14	B	1226	CLA	C1D-CHD-C4C	2.51	126.50	122.60
14	B	1201	CLA	CAA-C2A-C3A	-2.51	107.10	113.04
14	B	1229	CLA	C1D-C2D-C3D	-2.51	104.73	106.78
14	J	1302	CLA	C2D-C1D-ND	2.51	111.31	109.41
14	A	1011	CLA	C1D-CHD-C4C	2.51	126.49	122.60
14	B	1221	CLA	C1-C2-C3	2.51	130.65	126.19
14	A	1402	CLA	C2A-C3A-C4A	2.51	105.26	101.40
14	A	1140	CLA	O2D-CGD-CBD	2.51	116.44	111.33
14	B	1216	CLA	CED-O2D-CGD	2.51	121.99	116.02
14	A	1104	CLA	C2A-C1A-CHA	2.51	128.18	123.83
14	B	1235	CLA	C1D-CHD-C4C	2.51	126.49	122.60
14	F	1301	CLA	OBD-CAD-CBD	-2.51	122.16	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1210	CLA	C1D-CHD-C4C	2.50	126.48	122.60
17	A	4011	BCR	C30-C25-C26	-2.50	118.98	122.60
14	A	1237	CLA	C1D-CHD-C4C	2.50	126.48	122.60
14	B	1203	CLA	O2D-CGD-CBD	2.50	116.43	111.33
14	B	1233	CLA	OBD-CAD-CBD	-2.50	122.17	125.94
14	A	1801	CLA	CED-O2D-CGD	2.50	121.97	116.02
14	A	1134	CLA	CED-O2D-CGD	2.50	121.96	116.02
14	A	1112	CLA	C1D-CHD-C4C	2.50	126.47	122.60
14	B	1203	CLA	C1D-C2D-C3D	-2.49	104.74	106.78
14	A	1134	CLA	C1D-C2D-C3D	-2.49	104.74	106.78
14	B	1221	CLA	C2D-C1D-ND	2.49	111.29	109.41
14	B	1218	CLA	O1D-CGD-CBD	-2.49	119.31	124.42
14	B	1208	CLA	O2D-CGD-CBD	2.49	116.41	111.33
17	A	4002	BCR	C7-C8-C9	2.49	129.94	126.22
14	A	1136	CLA	C2D-C1D-ND	2.49	111.29	109.41
14	A	1103	CLA	C1D-C2D-C3D	-2.49	104.75	106.78
14	A	1115	CLA	C1D-CHD-C4C	2.49	126.46	122.60
14	A	1013	CLA	C2A-C3A-C4A	2.49	105.23	101.40
14	A	1118	CLA	C1D-C2D-C3D	-2.49	104.75	106.78
14	B	1209	CLA	C2D-C1D-ND	2.49	111.29	109.41
14	B	1206	CLA	CAA-C2A-C3A	-2.49	107.16	113.04
17	A	4011	BCR	C23-C22-C21	-2.49	115.15	118.97
17	L	4022	BCR	C1-C6-C5	-2.49	119.00	122.60
14	B	1225	CLA	CED-O2D-CGD	2.49	121.94	116.02
14	A	1117	CLA	C1D-C2D-C3D	-2.49	104.75	106.78
14	A	1135	CLA	C1D-C2D-C3D	-2.49	104.75	106.78
14	B	1239	CLA	C3B-CAB-CBB	-2.49	120.80	125.95
14	A	1801	CLA	C1D-C2D-C3D	-2.49	104.75	106.78
14	B	1234	CLA	OBD-CAD-CBD	-2.49	122.19	125.94
14	A	1107	CLA	CAA-C2A-C1A	2.48	117.83	111.62
17	M	4021	BCR	C30-C25-C26	-2.48	119.00	122.60
14	B	1211	CLA	C1D-CHD-C4C	2.48	126.45	122.60
14	B	1214	CLA	O2D-CGD-CBD	2.48	116.38	111.33
14	A	1131	CLA	C2A-C3A-C4A	2.48	105.21	101.40
14	B	1228	CLA	C1D-CHD-C4C	2.48	126.44	122.60
14	B	1207	CLA	OBD-CAD-CBD	-2.48	122.20	125.94
17	I	4018	BCR	C29-C30-C25	2.48	114.56	110.44
14	A	1117	CLA	O2D-CGD-CBD	2.47	116.37	111.33
14	B	1021	CLA	C1D-CHD-C4C	2.47	126.44	122.60
17	B	4006	BCR	C35-C13-C12	2.47	122.09	118.09
14	A	1113	CLA	C1D-C2D-C3D	-2.47	104.76	106.78
14	A	1115	CLA	C1D-C2D-C3D	-2.47	104.76	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4002	BCR	C24-C23-C22	2.47	129.91	126.22
14	B	1235	CLA	CAA-C2A-C3A	-2.47	107.20	113.04
17	J	4013	BCR	C1-C6-C5	-2.47	119.02	122.60
14	B	1210	CLA	CED-O2D-CGD	2.47	121.89	116.02
14	B	1217	CLA	C1-O2A-CGA	2.47	117.95	115.06
14	B	1218	CLA	C1D-C2D-C3D	-2.47	104.77	106.78
17	A	4002	BCR	C1-C6-C5	-2.46	119.03	122.60
14	A	1125	CLA	O1D-CGD-CBD	-2.46	119.37	124.42
14	A	1117	CLA	C4B-C3B-CAB	2.46	132.17	127.18
14	A	1135	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
14	B	1217	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
14	A	1110	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
14	B	1235	CLA	C1-C2-C3	2.46	130.56	126.19
14	J	1302	CLA	CBD-CHA-C1A	2.46	131.99	128.77
14	A	1124	CLA	C1-C2-C3	2.46	130.56	126.19
14	A	1113	CLA	CAA-C2A-C3A	-2.46	107.23	113.04
14	L	1501	CLA	O1D-CGD-CBD	-2.46	119.39	124.42
14	A	1140	CLA	CMB-C2B-C3B	2.46	128.84	124.97
17	J	4013	BCR	C23-C24-C25	2.46	134.57	127.32
14	A	1129	CLA	CED-O2D-CGD	2.46	121.86	116.02
14	A	1013	CLA	C1D-CHD-C4C	2.45	126.41	122.60
14	A	1022	CLA	O2A-CGA-CBA	2.45	119.66	111.94
14	A	1125	CLA	C2A-C3A-C4A	2.45	105.17	101.40
14	A	1801	CLA	C4D-CHA-CBD	-2.45	103.59	109.37
17	I	4018	BCR	C1-C6-C5	-2.45	119.05	122.60
17	J	4013	BCR	C36-C18-C19	2.45	122.05	118.09
14	B	1207	CLA	CED-O2D-CGD	2.45	121.84	116.02
14	B	1224	CLA	C1D-C2D-C3D	-2.45	104.78	106.78
14	A	1138	CLA	CAA-C2A-C3A	-2.44	107.26	113.04
14	A	1105	CLA	CED-O2D-CGD	2.44	121.82	116.02
14	B	1236	CLA	C1D-C2D-C3D	-2.44	104.79	106.78
14	A	1128	CLA	C3B-C2B-C1B	2.44	108.43	107.00
14	A	1119	CLA	O2A-CGA-CBA	2.44	119.61	111.94
14	B	1223	CLA	C1-C2-C3	2.44	130.52	126.19
14	A	1104	CLA	O2A-CGA-O1A	-2.44	116.78	123.43
14	B	1204	CLA	CMB-C2B-C1B	-2.43	124.88	128.62
14	B	1213	CLA	C1D-CHD-C4C	2.43	126.37	122.60
14	A	1109	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
17	B	4010	BCR	C32-C1-C6	2.43	114.36	110.33
14	A	1114	CLA	CMB-C2B-C3B	2.43	128.80	124.97
14	B	1209	CLA	CED-O2D-CGD	2.43	121.80	116.02
14	B	1227	CLA	C2D-C1D-ND	2.43	111.25	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1211	CLA	C2D-C1D-ND	2.43	111.25	109.41
14	B	1236	CLA	C3B-CAB-CBB	-2.43	120.92	125.95
17	B	4005	BCR	C32-C1-C6	2.43	114.35	110.33
14	A	1111	CLA	CED-O2D-CGD	2.43	121.79	116.02
14	A	1126	CLA	O2D-CGD-CBD	2.43	116.27	111.33
17	L	4019	BCR	C29-C30-C25	2.43	114.47	110.44
14	B	1214	CLA	C2A-C3A-C4A	2.43	105.13	101.40
14	X	1701	CLA	C2A-C3A-C4A	2.42	105.13	101.40
14	A	1140	CLA	C1D-C2D-C3D	-2.42	104.80	106.78
14	A	1123	CLA	C1D-CHD-C4C	2.42	126.36	122.60
14	A	1107	CLA	C1D-C2D-C3D	-2.42	104.80	106.78
17	B	4014	BCR	C35-C13-C12	2.43	122.01	118.09
17	B	4017	BCR	C34-C9-C8	2.43	122.01	118.09
14	B	1021	CLA	C4D-CHA-CBD	-2.42	103.67	109.37
17	A	4007	BCR	C1-C6-C7	2.42	122.40	115.69
14	B	1216	CLA	C1-C2-C3	2.42	130.49	126.19
14	B	1218	CLA	C2C-C1C-NC	-2.42	108.21	110.17
14	B	1224	CLA	C1-C2-C3	2.42	130.49	126.19
14	B	1230	CLA	C1D-CHD-C4C	2.42	126.35	122.60
14	B	1232	CLA	C2A-C3A-C4A	2.42	105.12	101.40
14	A	1138	CLA	C1D-C2D-C3D	-2.42	104.81	106.78
14	B	1239	CLA	C1D-C2D-C3D	-2.42	104.81	106.78
14	B	1205	CLA	CMB-C2B-C3B	2.42	128.78	124.97
17	J	4013	BCR	C28-C27-C26	2.42	117.40	113.74
14	B	1226	CLA	O1D-CGD-CBD	-2.41	119.47	124.42
14	A	1137	CLA	C1D-CHD-C4C	2.41	126.34	122.60
14	B	1228	CLA	CED-O2D-CGD	2.41	121.76	116.02
14	A	1119	CLA	C2D-C1D-ND	2.41	111.23	109.41
17	A	4001	BCR	C1-C6-C7	2.41	122.37	115.69
14	A	1111	CLA	C2A-C3A-C4A	2.41	105.10	101.40
14	B	1226	CLA	C2A-C3A-C4A	2.41	105.10	101.40
14	A	1125	CLA	C1D-CHD-C4C	2.41	126.33	122.60
14	B	1225	CLA	O2D-CGD-CBD	2.41	116.24	111.33
14	A	1127	CLA	C2B-C3B-CAB	-2.41	122.40	127.33
14	A	1132	CLA	O1D-CGD-CBD	-2.41	119.49	124.42
14	A	1113	CLA	O1D-CGD-CBD	-2.40	119.50	124.42
14	B	1221	CLA	C2A-C1A-CHA	2.40	128.00	123.83
17	I	4020	BCR	C36-C18-C19	2.40	121.98	118.09
14	A	1122	CLA	C1D-CHD-C4C	2.40	126.33	122.60
17	F	4016	BCR	C7-C8-C9	2.40	129.81	126.22
14	A	1120	CLA	CED-O2D-CGD	2.40	121.73	116.02
17	J	4015	BCR	C30-C25-C24	2.40	122.34	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	4012	BCR	C24-C23-C22	2.40	129.80	126.22
14	A	1140	CLA	C1D-CHD-C4C	2.40	126.31	122.60
14	A	1011	CLA	C1-C2-C3	2.39	130.44	126.19
14	B	1232	CLA	CMB-C2B-C3B	2.39	128.74	124.97
14	A	1106	CLA	C2C-C1C-NC	-2.39	108.23	110.17
14	A	1108	CLA	C1D-CHD-C4C	2.39	126.31	122.60
14	B	1222	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
14	B	1021	CLA	C2A-C3A-C4A	2.39	105.08	101.40
14	A	1107	CLA	CMB-C2B-C3B	2.39	128.74	124.97
14	A	1105	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
14	A	1132	CLA	CMB-C2B-C1B	-2.39	124.94	128.62
14	B	1204	CLA	C2D-C1D-ND	2.39	111.22	109.41
14	A	1133	CLA	CMB-C2B-C3B	2.39	128.73	124.97
14	B	1201	CLA	O1D-CGD-CBD	-2.39	119.53	124.42
14	B	1211	CLA	C2A-C3A-C4A	2.39	105.07	101.40
14	A	1105	CLA	C1D-C2D-C3D	-2.38	104.83	106.78
14	A	1115	CLA	OBD-CAD-CBD	-2.38	122.34	125.94
14	A	1106	CLA	C1D-CHD-C4C	2.38	126.30	122.60
14	B	1023	CLA	C1D-C2D-C3D	-2.38	104.84	106.78
14	A	1108	CLA	CMB-C2B-C3B	2.38	128.72	124.97
14	B	1233	CLA	C2A-C3A-C4A	2.38	105.06	101.40
14	B	1219	CLA	OBD-CAD-CBD	-2.38	122.35	125.94
17	A	4008	BCR	C8-C9-C10	-2.38	115.32	118.97
14	A	1111	CLA	C1-C2-C3	2.38	130.41	126.19
14	A	1102	CLA	OBD-CAD-CBD	-2.38	122.35	125.94
14	A	1113	CLA	CED-O2D-CGD	2.38	121.67	116.02
14	B	1203	CLA	CBD-CHA-C1A	2.38	131.88	128.77
14	A	1133	CLA	C1D-C2D-C3D	-2.38	104.84	106.78
14	A	1109	CLA	C1D-CHD-C4C	2.38	126.28	122.60
17	J	4012	BCR	C35-C13-C12	2.38	121.94	118.09
14	L	1502	CLA	C2A-C3A-C4A	2.38	105.06	101.40
14	A	1134	CLA	OBD-CAD-CBD	-2.37	122.35	125.94
14	B	1212	CLA	C1D-CHD-C4C	2.37	126.28	122.60
14	A	1121	CLA	C1D-CHD-C4C	2.38	126.28	122.60
14	B	1023	CLA	C2A-C3A-C4A	2.37	105.05	101.40
14	A	1138	CLA	OBD-CAD-CBD	-2.37	122.36	125.94
14	A	1105	CLA	C1-C2-C3	2.37	130.41	126.19
14	A	1129	CLA	C1-C2-C3	2.37	130.40	126.19
17	M	4021	BCR	C8-C7-C6	2.37	134.33	127.32
14	A	1801	CLA	C2A-C1A-CHA	2.37	127.94	123.83
14	B	1215	CLA	CED-O2D-CGD	2.37	121.66	116.02
14	B	1238	CLA	CMB-C2B-C3B	2.37	128.70	124.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1104	CLA	C2D-C1D-ND	2.37	111.20	109.41
14	B	1213	CLA	CMB-C2B-C3B	2.37	128.70	124.97
14	A	1130	CLA	C4B-C3B-CAB	2.37	131.97	127.18
17	A	4008	BCR	C37-C22-C23	2.36	121.91	118.09
14	B	1207	CLA	CMB-C2B-C1B	-2.36	124.99	128.62
14	A	1103	CLA	O1D-CGD-CBD	-2.36	119.58	124.42
14	L	1501	CLA	C1D-CHD-C4C	2.36	126.26	122.60
14	B	1222	CLA	O1D-CGD-CBD	-2.36	119.58	124.42
17	A	4002	BCR	C1-C6-C7	2.36	122.23	115.69
17	B	4009	BCR	C30-C25-C26	-2.36	119.18	122.60
14	B	1201	CLA	CBD-CHA-C1A	2.36	131.85	128.77
14	A	1119	CLA	C2A-C3A-C4A	2.36	105.03	101.40
14	A	1137	CLA	CED-O2D-CGD	2.36	121.62	116.02
14	B	1229	CLA	C1-C2-C3	2.36	130.38	126.19
14	A	1237	CLA	O2D-CGD-CBD	2.36	116.13	111.33
14	B	1207	CLA	C3A-C2A-C1A	2.36	104.41	101.08
14	A	1118	CLA	C2A-C3A-C4A	2.35	105.02	101.40
14	B	1201	CLA	C1D-CHD-C4C	2.36	126.25	122.60
14	B	1214	CLA	CBD-CHA-C1A	2.35	131.85	128.77
14	A	1109	CLA	C1D-C2D-C3D	-2.35	104.86	106.78
17	B	4006	BCR	C23-C24-C25	2.35	134.27	127.32
14	B	1239	CLA	C1D-CHD-C4C	2.35	126.25	122.60
14	F	1301	CLA	C2A-C1A-CHA	2.35	127.90	123.83
17	B	4014	BCR	C23-C24-C25	2.35	134.26	127.32
14	B	1236	CLA	CMB-C2B-C3B	2.35	128.67	124.97
17	L	4019	BCR	C36-C18-C19	2.35	121.89	118.09
14	A	1132	CLA	CED-O2D-CGD	2.35	121.60	116.02
14	A	1139	CLA	C1-C2-C3	2.35	130.36	126.19
14	A	1107	CLA	OBD-CAD-CBD	-2.35	122.40	125.94
14	A	1104	CLA	OBD-CAD-CBD	-2.35	122.40	125.94
14	A	1133	CLA	OBD-CAD-CBD	-2.35	122.40	125.94
14	J	1302	CLA	C2A-C1A-CHA	2.34	127.89	123.83
14	X	1701	CLA	CMB-C2B-C3B	2.34	128.66	124.97
14	A	1132	CLA	C1D-CHD-C4C	2.34	126.23	122.60
14	A	1140	CLA	C1-C2-C3	2.34	130.35	126.19
14	B	1217	CLA	O1D-CGD-CBD	-2.34	119.62	124.42
14	B	1223	CLA	C2A-C3A-C4A	2.34	105.00	101.40
14	B	1226	CLA	C1D-C2D-C3D	-2.34	104.87	106.78
17	A	4007	BCR	C32-C1-C6	2.34	114.20	110.33
14	A	1113	CLA	OBD-CAD-CBD	-2.34	122.41	125.94
14	B	1213	CLA	CED-O2D-CGD	2.34	121.58	116.02
14	B	1236	CLA	C1D-CHD-C4C	2.34	126.22	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1237	CLA	C2A-C3A-C4A	2.34	104.99	101.40
14	B	1021	CLA	CMB-C2B-C1B	-2.33	125.03	128.62
14	A	1124	CLA	C1D-CHD-C4C	2.33	126.22	122.60
14	B	1226	CLA	CAA-C2A-C3A	-2.33	107.53	113.04
14	A	1801	CLA	CMB-C2B-C3B	2.33	128.64	124.97
14	B	1202	CLA	CED-O2D-CGD	2.33	121.57	116.02
17	A	4011	BCR	C1-C6-C5	-2.33	119.22	122.60
14	L	1503	CLA	CMB-C2B-C3B	2.33	128.64	124.97
14	B	1211	CLA	CED-O2D-CGD	2.33	121.56	116.02
14	A	1121	CLA	CMB-C2B-C3B	2.33	128.64	124.97
14	B	1207	CLA	C1-C2-C3	2.33	130.32	126.19
17	I	4018	BCR	C30-C25-C26	-2.33	119.23	122.60
14	B	1217	CLA	C2A-C1A-CHA	2.33	127.86	123.83
17	B	4010	BCR	C1-C6-C5	-2.33	119.23	122.60
14	A	1124	CLA	CAA-C2A-C3A	-2.32	107.55	113.04
17	B	4017	BCR	C24-C23-C22	2.32	129.69	126.22
17	B	4014	BCR	C36-C18-C19	2.32	121.85	118.09
14	B	1204	CLA	CAA-C2A-C3A	-2.32	107.55	113.04
14	B	1236	CLA	CED-O2D-CGD	2.32	121.54	116.02
14	B	1225	CLA	C1D-C2D-C3D	-2.32	104.89	106.78
14	B	1214	CLA	C1-C2-C3	2.32	130.31	126.19
14	K	1401	CLA	CED-O2D-CGD	2.32	121.54	116.02
17	I	4020	BCR	C1-C6-C7	2.32	122.12	115.69
14	A	1130	CLA	OBD-CAD-CBD	-2.32	122.44	125.94
14	A	1119	CLA	CAA-CBA-CGA	2.32	120.74	113.27
14	A	1128	CLA	C1D-C2D-C3D	-2.32	104.89	106.78
14	B	1214	CLA	CMB-C2B-C3B	2.32	128.62	124.97
14	A	1127	CLA	CMD-C2D-C3D	2.32	128.62	124.97
14	A	1022	CLA	C1D-C2D-C3D	-2.31	104.89	106.78
17	A	4003	BCR	C28-C27-C26	2.31	117.24	113.74
14	A	1136	CLA	C1D-CHD-C4C	2.31	126.17	122.60
14	A	1105	CLA	C1D-CHD-C4C	2.31	126.17	122.60
14	B	1218	CLA	C2A-C1A-CHA	2.31	127.83	123.83
17	L	4022	BCR	C30-C25-C24	2.30	122.07	115.69
14	B	1225	CLA	C3A-C2A-C1A	2.30	104.33	101.08
14	B	1212	CLA	CMB-C2B-C3B	2.30	128.59	124.97
14	B	1215	CLA	C1D-C2D-C3D	-2.30	104.90	106.78
14	F	1301	CLA	CED-O2D-CGD	2.30	121.48	116.02
14	A	1126	CLA	CED-O2D-CGD	2.30	121.49	116.02
14	A	1123	CLA	CED-O2D-CGD	2.30	121.49	116.02
14	A	1122	CLA	C2A-C3A-C4A	2.30	104.94	101.40
14	A	1139	CLA	OBD-CAD-CBD	-2.30	122.47	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1135	CLA	C2A-C3A-C4A	2.30	104.93	101.40
14	A	1138	CLA	C2C-C1C-NC	-2.30	108.31	110.17
14	A	1127	CLA	C2A-C3A-C4A	2.30	104.93	101.40
14	A	1133	CLA	O2A-CGA-O1A	-2.29	117.16	123.43
14	B	1206	CLA	C1D-CHD-C4C	2.29	126.16	122.60
17	F	4016	BCR	C30-C25-C24	2.29	122.04	115.69
14	A	1123	CLA	C1D-C2D-C3D	-2.29	104.91	106.78
14	A	1120	CLA	CMB-C2B-C3B	2.29	128.58	124.97
14	B	1201	CLA	CMB-C2B-C3B	2.29	128.58	124.97
14	A	1106	CLA	CBD-CHA-C1A	2.29	131.76	128.77
14	B	1234	CLA	O1D-CGD-CBD	-2.29	119.73	124.42
17	A	4008	BCR	C34-C9-C8	2.29	121.79	118.09
14	B	1209	CLA	OBD-CAD-CBD	-2.29	122.48	125.94
14	A	1136	CLA	C1D-C2D-C3D	-2.29	104.91	106.78
14	A	1133	CLA	CAA-C2A-C3A	-2.29	107.64	113.04
18	A	5003	LHG	O10-C23-C24	-2.29	119.80	124.28
17	I	4020	BCR	C1-C6-C5	-2.28	119.29	122.60
14	A	1120	CLA	C1D-C2D-C3D	-2.28	104.92	106.78
14	B	1232	CLA	C2A-C1A-CHA	2.28	127.79	123.83
14	A	1013	CLA	C1-C2-C3	2.28	130.24	126.19
17	B	4004	BCR	C1-C6-C7	2.28	122.02	115.69
14	A	1109	CLA	O2D-CGD-CBD	2.28	115.98	111.33
14	B	1223	CLA	C1D-CHD-C4C	2.28	126.14	122.60
14	B	1206	CLA	CMB-C2B-C3B	2.28	128.56	124.97
14	B	1238	CLA	O2D-CGD-CBD	2.28	115.98	111.33
14	B	1210	CLA	OBD-CAD-CBD	-2.28	122.50	125.94
17	B	4009	BCR	C30-C25-C24	2.28	122.01	115.69
14	B	1204	CLA	CED-O2D-CGD	2.28	121.44	116.02
14	B	1232	CLA	CAA-C2A-C3A	-2.28	107.66	113.04
14	A	1120	CLA	C2C-C1C-NC	-2.28	108.32	110.17
14	B	1223	CLA	OBD-CAD-CBD	-2.28	122.50	125.94
17	A	4008	BCR	C23-C22-C21	-2.27	115.47	118.97
14	A	1140	CLA	C3A-C2A-C1A	2.28	104.30	101.08
14	X	1701	CLA	CBD-CHA-C1A	2.27	131.74	128.77
14	A	1110	CLA	C1D-C2D-C3D	-2.27	104.92	106.78
14	A	1113	CLA	C2A-C3A-C4A	2.27	104.89	101.40
14	A	1109	CLA	CMB-C2B-C3B	2.27	128.55	124.97
14	A	1102	CLA	C1D-CHD-C4C	2.27	126.12	122.60
17	B	4006	BCR	C30-C25-C24	2.27	121.98	115.69
14	A	1128	CLA	C2A-C3A-C4A	2.27	104.89	101.40
14	B	1226	CLA	O2A-CGA-O1A	-2.27	117.24	123.43
14	A	1137	CLA	C2D-C1D-ND	2.26	111.12	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1233	CLA	CED-O2D-CGD	2.26	121.40	116.02
14	A	1138	CLA	C1D-CHD-C4C	2.26	126.11	122.60
14	B	1225	CLA	CBA-CAA-C2A	2.26	120.73	114.01
14	B	1203	CLA	C1D-CHD-C4C	2.26	126.10	122.60
14	A	1127	CLA	CED-O2D-CGD	2.26	121.39	116.02
17	J	4013	BCR	C1-C6-C7	2.26	121.95	115.69
14	B	1208	CLA	C1D-C2D-C3D	-2.26	104.94	106.78
14	B	1217	CLA	CMB-C2B-C3B	2.26	128.52	124.97
14	B	1225	CLA	C1D-CHD-C4C	2.26	126.10	122.60
14	B	1202	CLA	C1D-CHD-C4C	2.26	126.10	122.60
17	J	4013	BCR	C24-C23-C22	2.26	129.59	126.22
14	B	1208	CLA	C2A-C3A-C4A	2.25	104.87	101.40
14	A	1122	CLA	C3B-CAB-CBB	-2.25	121.28	125.95
14	B	1217	CLA	CBD-CHA-C1A	2.26	131.72	128.77
17	A	4007	BCR	C1-C6-C5	-2.25	119.34	122.60
17	A	4007	BCR	C40-C30-C25	2.25	114.06	110.33
14	A	1128	CLA	CED-O2D-CGD	2.25	121.38	116.02
14	A	1237	CLA	CED-O2D-CGD	2.25	121.38	116.02
14	A	1137	CLA	C2A-C3A-C4A	2.25	104.86	101.40
17	I	4018	BCR	C1-C6-C7	2.25	121.92	115.69
14	B	1201	CLA	C5-C6-C7	-2.25	109.02	113.25
14	A	1109	CLA	C1-C2-C3	2.25	130.18	126.19
14	J	1302	CLA	CMB-C2B-C3B	2.25	128.51	124.97
14	B	1023	CLA	C1D-CHD-C4C	2.25	126.08	122.60
14	B	1203	CLA	CED-O2D-CGD	2.25	121.36	116.02
14	A	1126	CLA	C1D-CHD-C4C	2.24	126.08	122.60
14	B	1209	CLA	C2A-C3A-C4A	2.24	104.85	101.40
17	B	4017	BCR	C23-C22-C21	-2.24	115.52	118.97
17	I	4018	BCR	C19-C18-C17	-2.24	115.52	118.97
14	B	1226	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
14	A	1134	CLA	CMB-C2B-C3B	2.24	128.49	124.97
14	B	1221	CLA	C2A-C3A-C4A	2.24	104.84	101.40
14	A	1127	CLA	C4B-C3B-CAB	2.24	131.71	127.18
14	A	1118	CLA	C2C-C1C-NC	-2.24	108.36	110.17
17	I	4020	BCR	C19-C18-C17	-2.23	115.54	118.97
14	A	1125	CLA	OBD-CAD-CBD	-2.23	122.57	125.94
14	A	1402	CLA	CMB-C2B-C3B	2.23	128.49	124.97
14	B	1216	CLA	CMB-C2B-C3B	2.23	128.49	124.97
14	A	1108	CLA	C1D-C2D-C3D	-2.23	104.96	106.78
14	A	1131	CLA	C4B-C3B-CAB	2.23	131.69	127.18
14	A	1116	CLA	C2A-C3A-C4A	2.23	104.83	101.40
14	A	1117	CLA	O2A-CGA-O1A	-2.23	117.34	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1114	CLA	CBD-CHA-C1A	2.23	131.69	128.77
14	B	1227	CLA	C1C-NC-C4C	2.23	109.19	106.36
14	A	1120	CLA	O1D-CGD-CBD	-2.23	119.86	124.42
14	A	1103	CLA	C1-C2-C3	2.23	130.15	126.19
17	I	4020	BCR	C29-C30-C25	2.23	114.14	110.44
17	B	4010	BCR	C1-C6-C7	2.23	121.86	115.69
14	B	1227	CLA	CED-O2D-CGD	2.22	121.31	116.02
14	A	1137	CLA	C1D-C2D-C3D	-2.22	104.96	106.78
14	A	1139	CLA	C2A-C3A-C4A	2.22	104.82	101.40
14	A	1136	CLA	CAA-C2A-C3A	-2.22	107.78	113.04
14	A	1115	CLA	CMB-C2B-C3B	2.22	128.47	124.97
14	A	1011	CLA	CMB-C2B-C3B	2.22	128.47	124.97
14	A	1126	CLA	O2A-CGA-O1A	-2.22	117.37	123.43
14	J	1302	CLA	C2A-C3A-C4A	2.22	104.81	101.40
14	B	1012	CLA	CMB-C2B-C3B	2.22	128.46	124.97
14	B	1213	CLA	O2A-CGA-O1A	-2.22	117.38	123.43
17	L	4019	BCR	C1-C6-C5	-2.22	119.39	122.60
14	A	1022	CLA	C2A-C3A-C4A	2.22	104.81	101.40
14	B	1224	CLA	O1D-CGD-CBD	-2.22	119.88	124.42
14	A	1801	CLA	C2A-C3A-C4A	2.22	104.81	101.40
17	B	4017	BCR	C30-C25-C26	-2.22	119.39	122.60
14	B	1236	CLA	CAA-C2A-C3A	-2.22	107.80	113.04
14	A	1118	CLA	C2A-C1A-CHA	2.21	127.67	123.83
17	B	4006	BCR	C1-C6-C7	2.22	121.83	115.69
14	A	1122	CLA	CMB-C2B-C3B	2.21	128.46	124.97
14	A	1101	CLA	CMB-C2B-C3B	2.21	128.46	124.97
14	B	1206	CLA	C3B-C2B-C1B	2.21	108.30	107.00
14	B	1203	CLA	OBD-CAD-CBD	-2.21	122.60	125.94
14	B	1218	CLA	CMB-C2B-C3B	2.21	128.46	124.97
14	B	1208	CLA	C1D-CHD-C4C	2.21	126.03	122.60
17	B	4005	BCR	C35-C13-C12	2.21	121.67	118.09
14	B	1235	CLA	C2C-C1C-NC	-2.21	108.38	110.17
14	A	1119	CLA	O2D-CGD-CBD	2.21	115.84	111.33
14	B	1203	CLA	C2A-C3A-C4A	2.21	104.80	101.40
14	A	1139	CLA	C1D-C2D-C3D	-2.21	104.98	106.78
14	B	1233	CLA	C2A-C1A-CHA	2.21	127.66	123.83
14	B	1012	CLA	O2A-CGA-O1A	-2.21	117.40	123.43
14	A	1112	CLA	CAA-C2A-C3A	-2.21	107.82	113.04
14	B	1209	CLA	CMB-C2B-C3B	2.21	128.45	124.97
14	A	1106	CLA	O2A-CGA-O1A	-2.21	117.40	123.43
14	A	1402	CLA	CHA-C1A-NA	-2.21	122.82	125.56
17	A	4008	BCR	C7-C8-C9	2.21	129.52	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1235	CLA	C4-C3-C5	-2.21	112.03	115.39
14	B	1220	CLA	CMB-C2B-C3B	2.21	128.44	124.97
14	A	1116	CLA	CMB-C2B-C3B	2.21	128.44	124.97
14	B	1225	CLA	OBD-CAD-CBD	-2.20	122.61	125.94
14	A	1801	CLA	O2A-CGA-O1A	-2.20	117.41	123.43
14	A	1116	CLA	C3B-CAB-CBB	-2.20	121.39	125.95
14	B	1230	CLA	OBD-CAD-CBD	-2.20	122.61	125.94
14	A	1136	CLA	CED-O2D-CGD	2.20	121.26	116.02
14	B	1221	CLA	O1D-CGD-CBD	-2.20	119.91	124.42
17	J	4013	BCR	C40-C30-C25	2.20	113.98	110.33
14	A	1102	CLA	C2A-C3A-C4A	2.20	104.79	101.40
14	A	1101	CLA	C1D-C2D-C3D	-2.20	104.98	106.78
14	B	1221	CLA	C1D-C2D-C3D	-2.20	104.98	106.78
14	B	1227	CLA	C3B-CAB-CBB	-2.20	121.40	125.95
14	A	1118	CLA	O1D-CGD-CBD	-2.20	119.92	124.42
14	A	1122	CLA	C2D-C1D-ND	2.20	111.07	109.41
17	B	4014	BCR	C24-C23-C22	2.20	129.50	126.22
14	B	1234	CLA	C1D-C2D-C3D	-2.20	104.98	106.78
14	B	1220	CLA	C2A-C3A-C4A	2.20	104.78	101.40
14	A	1119	CLA	C2C-C1C-NC	-2.20	108.39	110.17
14	A	1116	CLA	CBD-CHA-C1A	2.20	131.64	128.77
14	B	1228	CLA	C2C-C1C-NC	-2.19	108.39	110.17
17	B	4005	BCR	C34-C9-C8	2.19	121.64	118.09
14	B	1224	CLA	OBD-CAD-C3D	2.19	131.99	127.91
14	A	1131	CLA	CAA-C2A-C3A	-2.19	107.86	113.04
14	A	1237	CLA	CMB-C2B-C3B	2.19	128.41	124.97
14	A	1022	CLA	CAA-C2A-C3A	-2.19	107.87	113.04
14	A	1109	CLA	C2A-C3A-C4A	2.19	104.76	101.40
14	A	1107	CLA	CAA-C2A-C3A	-2.19	107.87	113.04
14	A	1128	CLA	C1D-CHD-C4C	2.19	125.99	122.60
17	A	4011	BCR	C3-C4-C5	2.19	117.05	113.74
14	B	1222	CLA	C1D-C2D-C3D	-2.19	105.00	106.78
14	A	1801	CLA	OBD-CAD-CBD	-2.18	122.64	125.94
14	A	1128	CLA	C2C-C1C-NC	-2.19	108.40	110.17
14	B	1234	CLA	CED-O2D-CGD	2.19	121.22	116.02
14	A	1121	CLA	C2A-C3A-C4A	2.18	104.76	101.40
14	B	1227	CLA	OBD-CAD-CBD	-2.18	122.64	125.94
17	F	4016	BCR	C1-C6-C7	2.18	121.74	115.69
17	B	4005	BCR	C36-C18-C19	2.18	121.62	118.09
14	A	1114	CLA	C1D-C2D-C3D	-2.18	105.00	106.78
14	A	1118	CLA	O2A-CGA-O1A	-2.18	117.47	123.43
14	A	1112	CLA	O1D-CGD-CBD	-2.18	119.95	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1023	CLA	CBD-CHA-C1A	2.18	131.62	128.77
14	B	1206	CLA	C2A-C3A-C4A	2.18	104.75	101.40
14	B	1012	CLA	CHA-C1A-NA	-2.18	121.75	126.22
14	B	1201	CLA	C1-C2-C3	2.18	130.06	126.19
14	A	1122	CLA	C1D-C2D-C3D	-2.18	105.00	106.78
14	A	1112	CLA	C2A-C3A-C4A	2.18	104.75	101.40
14	B	1231	CLA	C1D-C2D-C3D	-2.18	105.00	106.78
14	A	1139	CLA	CMB-C2B-C3B	2.18	128.40	124.97
14	B	1233	CLA	CBD-CHA-C1A	2.18	131.61	128.77
14	B	1217	CLA	C2A-C3A-C4A	2.18	104.75	101.40
14	M	1601	CLA	C2A-C1A-CHA	2.18	127.60	123.83
14	K	1401	CLA	CMB-C2B-C3B	2.18	128.40	124.97
17	A	4008	BCR	C1-C6-C5	-2.17	119.45	122.60
14	B	1222	CLA	CED-O2D-CGD	2.17	121.19	116.02
14	B	1216	CLA	C2A-C3A-C4A	2.17	104.74	101.40
14	L	1503	CLA	C2A-C3A-C4A	2.17	104.74	101.40
14	A	1135	CLA	C2A-C1A-CHA	2.17	127.59	123.83
14	B	1215	CLA	O2A-CGA-O1A	-2.17	117.50	123.43
14	A	1134	CLA	CBD-CHA-C1A	2.17	131.60	128.77
17	I	4018	BCR	C34-C9-C8	2.17	121.60	118.09
14	A	1139	CLA	C3B-CAB-CBB	-2.17	121.46	125.95
17	A	4002	BCR	C23-C24-C25	2.17	133.72	127.32
17	A	4001	BCR	C37-C22-C23	2.16	121.59	118.09
17	A	4001	BCR	C35-C13-C12	2.16	121.59	118.09
14	B	1235	CLA	C2D-C1D-ND	2.16	111.05	109.41
14	L	1502	CLA	CMB-C2B-C3B	2.16	128.38	124.97
14	A	1127	CLA	C1D-C2D-C3D	-2.17	105.01	106.78
14	B	1213	CLA	C1D-C2D-C3D	-2.16	105.01	106.78
14	A	1134	CLA	C2A-C1A-CHA	2.16	127.58	123.83
14	A	1133	CLA	C2A-C3A-C4A	2.16	104.73	101.40
14	B	1209	CLA	C1D-C2D-C3D	-2.16	105.01	106.78
14	A	1125	CLA	C2C-C1C-NC	-2.16	108.42	110.17
14	A	1116	CLA	C2C-C1C-NC	-2.16	108.42	110.17
14	A	1101	CLA	C1-C2-C3	2.16	130.03	126.19
14	A	1121	CLA	C2D-C1D-ND	2.16	111.04	109.41
14	A	1120	CLA	C1C-NC-C4C	2.16	109.10	106.36
14	B	1218	CLA	C1C-NC-C4C	2.16	109.11	106.36
14	B	1231	CLA	CBD-CHA-C1A	2.16	131.59	128.77
14	A	1118	CLA	CED-O2D-CGD	2.16	121.15	116.02
14	A	1138	CLA	CMB-C2B-C3B	2.16	128.36	124.97
17	L	4019	BCR	C28-C27-C26	2.16	117.01	113.74
17	B	4006	BCR	C34-C9-C8	2.16	121.58	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1119	CLA	C11-C12-C13	2.16	121.35	115.14
17	B	4006	BCR	C36-C18-C19	2.15	121.58	118.09
14	A	1801	CLA	CAA-C2A-C3A	-2.15	107.95	113.04
17	A	4011	BCR	C34-C9-C8	2.15	121.57	118.09
14	A	1138	CLA	O2D-CGD-CBD	2.15	115.72	111.33
14	A	1102	CLA	CBD-CHA-C1A	2.15	131.58	128.77
17	B	4009	BCR	C36-C18-C19	2.15	121.57	118.09
14	A	1119	CLA	C12-C11-C10	-2.15	101.97	113.02
14	B	1228	CLA	CMB-C2B-C3B	2.15	128.36	124.97
14	A	1111	CLA	C2A-C1A-CHA	2.15	127.56	123.83
17	A	4007	BCR	C23-C24-C25	2.15	133.67	127.32
14	B	1233	CLA	C1D-C2D-C3D	-2.15	105.03	106.78
14	A	1013	CLA	C1-O2A-CGA	2.15	123.00	116.98
14	A	1112	CLA	C2A-C1A-CHA	2.15	127.56	123.83
14	B	1227	CLA	C2A-C3A-C4A	2.15	104.70	101.40
14	A	1137	CLA	C1-O2A-CGA	2.15	117.58	115.06
14	B	1206	CLA	CBD-CHA-C1A	2.15	131.58	128.77
14	B	1208	CLA	CMB-C2B-C3B	2.15	128.35	124.97
14	B	1229	CLA	CMB-C2B-C3B	2.15	128.35	124.97
14	B	1232	CLA	C1D-C2D-C3D	-2.15	105.03	106.78
14	B	1210	CLA	C2A-C1A-CHA	2.15	127.55	123.83
14	A	1801	CLA	C2A-C1A-NA	-2.15	108.87	111.24
14	A	1237	CLA	CMA-C3A-C2A	-2.15	104.92	114.14
14	A	1135	CLA	C4D-CHA-CBD	-2.15	104.32	109.37
14	B	1235	CLA	C1D-C2D-C3D	-2.14	105.03	106.78
17	J	4012	BCR	C37-C22-C23	2.14	121.56	118.09
14	A	1105	CLA	C2A-C3A-C4A	2.14	104.70	101.40
14	F	1301	CLA	C2A-C3A-C4A	2.14	104.70	101.40
14	A	1101	CLA	CAA-C2A-C3A	-2.14	107.97	113.04
14	B	1023	CLA	OBD-CAD-C3D	2.14	131.89	127.91
17	M	4021	BCR	C30-C25-C24	2.14	121.62	115.69
17	B	4014	BCR	C1-C6-C5	-2.14	119.50	122.60
14	A	1116	CLA	CBA-CAA-C2A	2.14	120.36	114.01
14	B	1230	CLA	C2C-C1C-NC	-2.14	108.44	110.17
17	B	4017	BCR	C1-C6-C5	-2.14	119.51	122.60
14	A	1138	CLA	C2A-C3A-C4A	2.13	104.68	101.40
14	A	1102	CLA	C2A-C1A-CHA	2.13	127.53	123.83
14	A	1022	CLA	C2C-C1C-NC	-2.13	108.44	110.17
14	A	1123	CLA	C2A-C1A-CHA	2.13	127.52	123.83
14	B	1207	CLA	O1D-CGD-CBD	-2.13	120.06	124.42
14	F	1301	CLA	CBD-CHA-C1A	2.13	131.55	128.77
14	B	1232	CLA	C3B-C2B-C1B	2.13	108.25	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	4013	BCR	C34-C9-C8	2.13	121.53	118.09
17	J	4013	BCR	C35-C13-C12	2.13	121.53	118.09
14	B	1223	CLA	O1D-CGD-CBD	-2.13	120.06	124.42
14	B	1234	CLA	C2A-C3A-C4A	2.13	104.67	101.40
14	X	1701	CLA	C2C-C1C-NC	-2.13	108.45	110.17
17	J	4013	BCR	C19-C18-C17	-2.13	115.70	118.97
14	B	1224	CLA	CMB-C2B-C3B	2.12	128.32	124.97
17	A	4001	BCR	C30-C25-C24	2.12	121.58	115.69
14	A	1109	CLA	C4D-CHA-CBD	-2.12	104.37	109.37
14	A	1139	CLA	CED-O2D-CGD	2.12	121.07	116.02
14	A	1117	CLA	C1-C2-C3	2.12	129.96	126.19
14	B	1225	CLA	CMB-C2B-C3B	2.12	128.31	124.97
14	A	1140	CLA	C1-O2A-CGA	2.12	122.92	116.98
14	B	1226	CLA	CED-O2D-CGD	2.12	121.06	116.02
17	B	4010	BCR	C19-C18-C17	-2.12	115.71	118.97
14	A	1104	CLA	C4D-CHA-CBD	-2.12	104.38	109.37
14	X	1701	CLA	CED-O2D-CGD	2.12	121.06	116.02
14	A	1129	CLA	C2A-C3A-C4A	2.12	104.66	101.40
14	A	1120	CLA	C2A-C1A-CHA	2.12	127.50	123.83
17	B	4004	BCR	C8-C7-C6	2.12	133.57	127.32
14	A	1022	CLA	C1D-CHD-C4C	2.12	125.88	122.60
14	B	1232	CLA	O2D-CGD-CBD	2.12	115.64	111.33
14	B	1211	CLA	C1D-C2D-C3D	-2.12	105.05	106.78
14	A	1135	CLA	C1D-CHD-C4C	2.12	125.88	122.60
14	A	1118	CLA	C1C-NC-C4C	2.11	109.05	106.36
14	A	1112	CLA	CMB-C2B-C3B	2.12	128.30	124.97
14	B	1239	CLA	CBA-CAA-C2A	2.11	120.29	114.01
14	A	1116	CLA	C1-C2-C3	2.11	129.94	126.19
17	A	4001	BCR	C32-C1-C6	2.11	113.83	110.33
14	B	1012	CLA	C2A-C3A-C4A	2.11	104.65	101.40
14	B	1222	CLA	C1C-NC-C4C	2.11	109.04	106.36
14	B	1211	CLA	CMB-C2B-C3B	2.11	128.29	124.97
14	B	1212	CLA	C2A-C3A-C4A	2.11	104.64	101.40
14	M	1601	CLA	CMB-C2B-C3B	2.11	128.29	124.97
17	B	4017	BCR	C30-C25-C24	2.11	121.53	115.69
14	A	1102	CLA	CED-O2D-CGD	2.11	121.03	116.02
14	A	1119	CLA	C1C-NC-C4C	2.11	109.04	106.36
14	B	1236	CLA	C2A-C3A-C4A	2.11	104.64	101.40
14	K	1401	CLA	OBD-CAD-CBD	-2.11	122.76	125.94
14	B	1012	CLA	O1D-CGD-CBD	-2.11	120.11	124.42
18	A	5003	LHG	C13-C12-C11	-2.11	109.73	114.46
14	A	1135	CLA	O1D-CGD-CBD	-2.10	120.11	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	1501	CLA	C3A-C2A-C1A	2.10	104.05	101.08
17	L	4019	BCR	C37-C22-C23	2.10	121.49	118.09
14	A	1112	CLA	C1D-C2D-C3D	-2.10	105.06	106.78
17	B	4017	BCR	C23-C24-C25	2.10	133.53	127.32
14	M	1601	CLA	C2A-C1A-NA	-2.10	108.92	111.24
17	B	4017	BCR	C15-C14-C13	2.10	130.32	127.29
14	K	1401	CLA	C2A-C3A-C4A	2.10	104.63	101.40
14	B	1220	CLA	C1D-C2D-C3D	-2.10	105.06	106.78
14	B	1218	CLA	C2A-C3A-C4A	2.10	104.63	101.40
14	B	1206	CLA	C12-C11-C10	-2.10	102.26	113.02
14	B	1203	CLA	CAA-C2A-C3A	-2.10	108.08	113.04
14	B	1205	CLA	C7-C6-C5	-2.10	106.83	113.01
14	B	1212	CLA	C2A-C1A-CHA	2.10	127.46	123.83
14	A	1134	CLA	C2C-C1C-NC	-2.09	108.47	110.17
14	A	1135	CLA	CBD-CHA-C1A	2.09	131.51	128.77
17	A	4011	BCR	C37-C22-C23	2.09	121.47	118.09
14	A	1130	CLA	CBD-CHA-C1A	2.09	131.50	128.77
14	B	1212	CLA	C4D-CHA-CBD	-2.09	104.45	109.37
17	A	4003	BCR	C35-C13-C12	2.09	121.47	118.09
14	A	1117	CLA	C2A-C1A-CHA	2.09	127.45	123.83
14	A	1135	CLA	C4B-C3B-CAB	2.09	131.41	127.18
14	A	1107	CLA	C2A-C1A-NA	-2.09	108.93	111.24
14	B	1217	CLA	C1D-C2D-C3D	-2.09	105.07	106.78
14	X	1701	CLA	C2A-C1A-CHA	2.09	127.45	123.83
14	A	1402	CLA	C1D-C2D-C3D	-2.09	105.08	106.78
14	A	1022	CLA	C2D-C1D-ND	2.09	110.99	109.41
14	A	1110	CLA	O2A-CGA-O1A	-2.09	117.73	123.43
17	B	4017	BCR	C11-C10-C9	2.09	130.30	127.29
14	A	1128	CLA	CBD-CHA-C1A	2.09	131.50	128.77
14	B	1215	CLA	C2A-C3A-C4A	2.09	104.61	101.40
14	B	1219	CLA	CBD-CHA-C1A	2.08	131.50	128.77
14	L	1501	CLA	C4-C3-C5	-2.08	112.22	115.39
14	F	1301	CLA	C1D-C2D-C3D	-2.08	105.08	106.78
14	B	1207	CLA	C4D-CHA-CBD	-2.08	104.47	109.37
14	A	1114	CLA	C2A-C1A-CHA	2.08	127.44	123.83
14	A	1129	CLA	O2A-CGA-O1A	-2.08	117.74	123.43
14	B	1209	CLA	C1C-NC-C4C	2.08	109.01	106.36
14	B	1212	CLA	C2C-C1C-NC	-2.08	108.48	110.17
17	M	4021	BCR	C35-C13-C12	2.08	121.46	118.09
14	J	1302	CLA	O1D-CGD-CBD	-2.08	120.16	124.42
17	A	4002	BCR	C40-C30-C25	2.08	113.77	110.33
14	A	1110	CLA	CED-O2D-CGD	2.08	120.96	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1210	CLA	C2A-C3A-C4A	2.08	104.59	101.40
17	B	4017	BCR	C28-C27-C26	2.08	116.89	113.74
14	A	1106	CLA	C2A-C3A-C4A	2.08	104.59	101.40
14	A	1113	CLA	C2A-C1A-CHA	2.07	127.42	123.83
14	B	1239	CLA	OBD-CAD-C3D	2.07	131.77	127.91
14	A	1129	CLA	C1C-NC-C4C	2.07	108.99	106.36
14	A	1106	CLA	C4D-CHA-CBD	-2.07	104.49	109.37
14	B	1214	CLA	C2A-C1A-CHA	2.07	127.42	123.83
14	B	1230	CLA	C2A-C3A-C4A	2.07	104.59	101.40
14	A	1126	CLA	CBD-CHA-C1A	2.07	131.48	128.77
14	B	1023	CLA	CAA-C2A-C3A	-2.07	108.15	113.04
14	A	1139	CLA	C2A-C1A-CHA	2.07	127.41	123.83
14	A	1130	CLA	O2A-CGA-O1A	-2.07	117.78	123.43
14	B	1221	CLA	C2C-C1C-NC	-2.07	108.50	110.17
17	B	4014	BCR	C28-C27-C26	2.07	116.87	113.74
14	A	1101	CLA	C2A-C1A-CHA	2.07	127.41	123.83
17	J	4013	BCR	C15-C14-C13	2.07	130.27	127.29
14	A	1139	CLA	CAA-C2A-C3A	-2.07	108.16	113.04
14	B	1226	CLA	CBD-CHA-C1A	2.06	131.47	128.77
17	J	4012	BCR	C19-C18-C17	-2.06	115.80	118.97
14	A	1117	CLA	CBA-CAA-C2A	2.06	120.13	114.01
14	X	1701	CLA	C1D-C2D-C3D	-2.06	105.10	106.78
14	B	1235	CLA	O1D-CGD-CBD	-2.06	120.20	124.42
17	B	4009	BCR	C28-C27-C26	2.06	116.86	113.74
14	A	1116	CLA	C2A-C1A-CHA	2.06	127.40	123.83
14	B	1229	CLA	C12-C11-C10	-2.06	102.47	113.02
14	A	1013	CLA	OBD-CAD-CBD	-2.06	122.83	125.94
17	B	4010	BCR	C34-C9-C8	2.06	121.42	118.09
17	B	4004	BCR	C20-C21-C22	2.06	130.25	127.29
17	A	4002	BCR	C15-C14-C13	2.05	130.25	127.29
14	L	1502	CLA	C2C-C1C-NC	-2.05	108.51	110.17
17	A	4003	BCR	C8-C7-C6	2.05	133.38	127.32
17	I	4018	BCR	C30-C25-C24	2.05	121.38	115.69
14	J	1303	CLA	C1D-C2D-C3D	-2.05	105.11	106.78
17	J	4015	BCR	C16-C17-C18	2.05	130.25	127.29
14	B	1208	CLA	C2C-C1C-NC	-2.05	108.51	110.17
14	A	1013	CLA	C4D-CHA-CBD	-2.05	104.55	109.37
14	B	1221	CLA	CMB-C2B-C3B	2.05	128.19	124.97
14	A	1123	CLA	C4D-CHA-CBD	-2.05	104.55	109.37
17	B	4006	BCR	C20-C21-C22	2.05	130.24	127.29
14	B	1217	CLA	C1C-NC-C4C	2.05	108.96	106.36
14	A	1128	CLA	O2A-CGA-O1A	-2.05	117.83	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1136	CLA	CMB-C2B-C3B	2.05	128.19	124.97
14	J	1303	CLA	CMB-C2B-C3B	2.05	128.19	124.97
14	A	1132	CLA	C5-C3-C2	2.05	125.02	121.08
14	B	1223	CLA	CED-O2D-CGD	2.05	120.89	116.02
14	A	1134	CLA	C2A-C3A-C4A	2.05	104.55	101.40
14	B	1222	CLA	C2A-C1A-NA	-2.04	108.98	111.24
14	B	1222	CLA	O2A-CGA-O1A	-2.04	118.73	122.96
14	B	1205	CLA	CED-O2D-CGD	2.05	120.89	116.02
14	B	1214	CLA	C1D-C2D-C3D	-2.05	105.11	106.78
14	A	1123	CLA	CBD-CHA-C1A	2.04	131.44	128.77
14	L	1502	CLA	C1D-CHD-C4C	2.04	125.77	122.60
14	J	1302	CLA	C4D-CHA-CBD	-2.04	104.56	109.37
17	B	4005	BCR	C15-C14-C13	2.04	130.23	127.29
14	A	1114	CLA	C4D-CHA-CBD	-2.04	104.56	109.37
17	B	4004	BCR	C34-C9-C8	2.04	121.39	118.09
14	B	1235	CLA	C1C-NC-C4C	2.04	108.95	106.36
17	B	4014	BCR	C30-C25-C24	2.04	121.35	115.69
14	A	1101	CLA	C2A-C3A-C4A	2.04	104.54	101.40
14	B	1230	CLA	CBA-CAA-C2A	2.04	120.06	114.01
14	B	1219	CLA	C1D-C2D-C3D	-2.04	105.12	106.78
14	B	1239	CLA	CED-O2D-CGD	2.04	120.87	116.02
14	B	1231	CLA	C1C-NC-C4C	2.04	108.95	106.36
14	A	1108	CLA	C2A-C3A-C4A	2.04	104.54	101.40
14	F	1301	CLA	CMB-C2B-C3B	2.04	128.18	124.97
14	B	1206	CLA	C1-C2-C3	2.04	129.81	126.19
14	A	1110	CLA	CAA-C2A-C3A	-2.04	108.22	113.04
17	B	4006	BCR	C40-C30-C25	2.04	113.70	110.33
14	B	1227	CLA	C2C-C1C-NC	-2.03	108.52	110.17
14	A	1125	CLA	O2A-CGA-O1A	-2.03	117.88	123.43
14	B	1202	CLA	CBD-CHA-C1A	2.03	131.43	128.77
14	A	1121	CLA	O2A-CGA-O1A	-2.03	117.88	123.43
14	A	1113	CLA	CBD-CHA-C1A	2.03	131.43	128.77
14	B	1222	CLA	C2A-C1A-CHA	2.03	127.35	123.83
17	J	4015	BCR	C3-C4-C5	2.03	116.82	113.74
14	A	1123	CLA	C1-C2-C3	2.03	129.80	126.19
14	J	1302	CLA	C1D-C2D-C3D	-2.03	105.12	106.78
14	A	1104	CLA	CAA-CBA-CGA	2.03	119.81	113.27
14	B	1023	CLA	C4D-CHA-CBD	-2.03	104.59	109.37
17	L	4019	BCR	C23-C24-C25	2.03	133.31	127.32
14	A	1022	CLA	CED-O2D-CGD	2.03	120.84	116.02
14	A	1117	CLA	C5-C3-C2	2.03	124.98	121.08
14	B	1021	CLA	C1D-C2D-C3D	-2.03	105.13	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1023	CLA	C1C-NC-C4C	2.02	108.93	106.36
14	A	1114	CLA	C2A-C3A-C4A	2.02	104.52	101.40
14	A	1136	CLA	O2D-CGD-CBD	2.02	115.46	111.33
14	A	1106	CLA	CED-O2D-CGD	2.02	120.83	116.02
14	B	1212	CLA	OBD-CAD-CBD	-2.02	122.88	125.94
14	M	1601	CLA	C1D-C2D-C3D	-2.03	105.13	106.78
17	F	4016	BCR	C36-C18-C19	2.02	121.36	118.09
17	B	4005	BCR	C30-C25-C24	2.02	121.29	115.69
17	B	4004	BCR	C37-C22-C23	2.02	121.36	118.09
14	A	1022	CLA	C6-C5-C3	-2.02	107.97	112.78
14	L	1502	CLA	C1C-NC-C4C	2.02	108.93	106.36
14	B	1209	CLA	CAA-C2A-C3A	-2.02	108.26	113.04
14	A	1104	CLA	C1D-C2D-C3D	-2.02	105.13	106.78
14	B	1206	CLA	C1D-C2D-C3D	-2.02	105.13	106.78
14	B	1207	CLA	CMB-C2B-C3B	2.02	128.15	124.97
14	B	1012	CLA	CAA-C2A-C3A	-2.02	108.26	113.04
14	A	1125	CLA	CMB-C2B-C3B	2.02	128.15	124.97
14	M	1601	CLA	C2A-C3A-C4A	2.02	104.51	101.40
14	B	1023	CLA	C2C-C1C-NC	-2.02	108.53	110.17
17	M	4021	BCR	C37-C22-C23	2.02	121.36	118.09
14	A	1140	CLA	CBA-CAA-C2A	2.02	120.01	114.01
14	A	1107	CLA	CBA-CAA-C2A	2.02	120.00	114.01
14	A	1113	CLA	C4D-CHA-CBD	-2.02	104.62	109.37
14	B	1204	CLA	C1-C2-C3	2.02	129.77	126.19
14	A	1137	CLA	CMB-C2B-C3B	2.01	128.14	124.97
17	L	4022	BCR	C1-C6-C7	2.02	121.27	115.69
14	B	1207	CLA	C2A-C1A-NA	-2.02	109.01	111.24
14	B	1201	CLA	C4D-CHA-CBD	-2.02	104.62	109.37
14	L	1502	CLA	O2A-CGA-O1A	-2.02	117.93	123.43
17	B	4009	BCR	C19-C18-C17	-2.02	115.87	118.97
14	A	1122	CLA	O2A-CGA-O1A	-2.02	117.92	123.43
14	B	1224	CLA	C2C-C1C-NC	-2.01	108.54	110.17
17	B	4014	BCR	C11-C10-C9	2.01	130.19	127.29
14	L	1501	CLA	C4D-CHA-CBD	-2.01	104.63	109.37
17	A	4002	BCR	C35-C13-C12	2.01	121.34	118.09
14	A	1131	CLA	CED-O2D-CGD	2.01	120.80	116.02
14	A	1107	CLA	C3A-C2A-C1A	2.01	103.92	101.08
17	B	4014	BCR	C40-C30-C25	2.01	113.66	110.33
14	B	1231	CLA	C2C-C1C-NC	-2.01	108.54	110.17
17	L	4022	BCR	C32-C1-C6	2.01	113.65	110.33
14	A	1118	CLA	CMB-C2B-C3B	2.01	128.13	124.97
14	A	1105	CLA	C2A-C1A-CHA	2.01	127.31	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	I	4020	BCR	C35-C13-C12	2.00	121.33	118.09
14	B	1236	CLA	O2A-CGA-O1A	-2.00	117.96	123.43
14	B	1218	CLA	C4D-CHA-CBD	-2.00	104.65	109.37
17	A	4008	BCR	C30-C25-C24	2.00	121.24	115.69
14	B	1204	CLA	OBD-CAD-C3D	2.00	131.63	127.91
14	A	1110	CLA	C2A-C3A-C4A	2.00	104.48	101.40
14	A	1107	CLA	O2A-CGA-O1A	-2.00	117.97	123.43
14	J	1302	CLA	C2C-C1C-NC	-2.00	108.55	110.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	5003	LHG	C2

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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