



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2014 – 05:26 AM GMT

PDB ID : 2PPS
Title : PHOTOSYNTHETIC REACTION CENTER AND CORE ANTENNA SYSTEM (TRIMERIC), ALPHA CARBON ONLY
Authors : Krauss, N.; Schubert, W.-D.; Klukas, O.; Fromme, P.; Witt, H.T.; Saenger, W.
Deposited on : 1997-05-27
Resolution : 4.00 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>

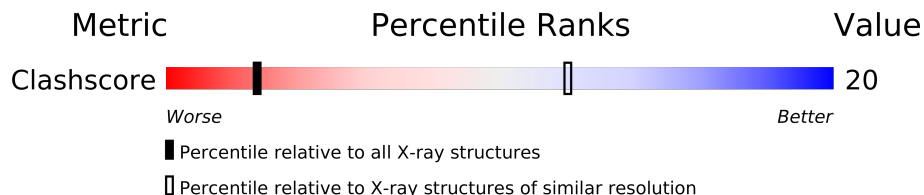
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 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) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 4.00 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	1235 (4.50-3.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	478	
2	B	503	
3	L	111	
4	K	64	
5	F	130	
6	C	80	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3616 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.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	478	Total	C	0	0	478
			478	478			

- Molecule 2 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	503	Total	C	0	0	503
			503	503			

- Molecule 3 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	L	111	Total	C	0	0	111
			111	111			

- Molecule 4 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	K	64	Total	C	0	0	64
			64	64			

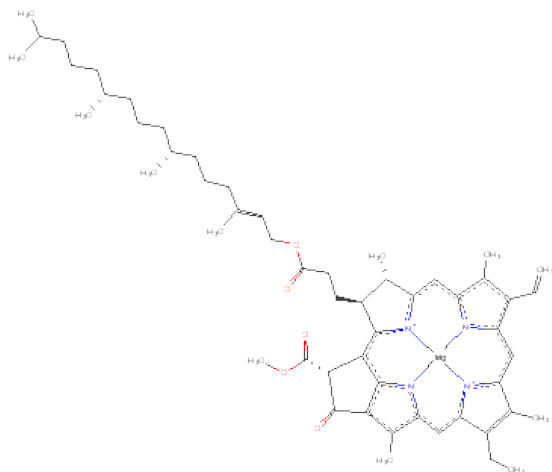
- Molecule 5 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	F	130	Total	C	0	0	130
			130	130			

- Molecule 6 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	C	80	Total	C	0	0	80
			80	80			

- Molecule 7 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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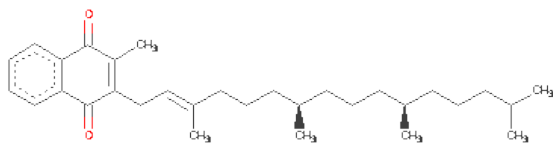
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

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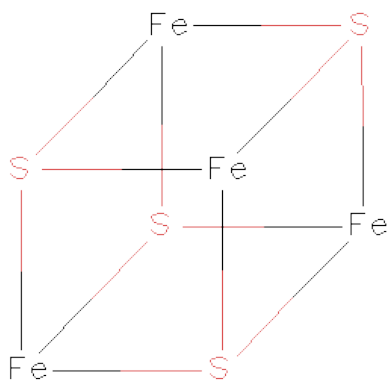
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25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

- Molecule 8 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	C	0	0
			1	1		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		

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

Chain A: 



- Molecule 2: PHOTOSYSTEM I

Chain B: 



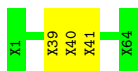
- Molecule 3: PHOTOSYSTEM I

Chain L: 

There are no outlier residues recorded for this chain.

- Molecule 4: PHOTOSYSTEM I

Chain K: 



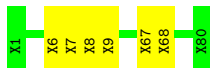
- Molecule 5: PHOTOSYSTEM I

Chain F: 



- Molecule 6: PHOTOSYSTEM I

Chain C: 



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	286.00Å 286.00Å 167.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-4.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
Refinement program	?	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3616	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	478	0	0	16	0
2	B	503	0	0	16	0
3	L	111	0	0	0	0
4	K	64	0	0	2	0
5	F	130	0	0	1	0
6	C	80	0	0	4	0
7	A	1000	0	120	41	0
7	B	850	0	102	12	0
7	F	225	0	27	8	0
7	K	50	0	6	0	0
7	L	100	0	12	0	0
8	B	1	0	0	0	0
9	B	8	0	0	3	0
9	C	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3616	0	267	78	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (78) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:A:3014:CLA:HHC	7:A:3029:CLA:C3D	1.61	1.31
1:A:94:UNK:CA	1:A:107:UNK:CA	2.11	1.29
2:B:470:UNK:CA	2:B:474:UNK:CA	2.12	1.27
1:A:295:UNK:CA	7:A:3016:CLA:C3C	2.19	1.20
2:B:428:UNK:CA	7:B:2005:CLA:C3A	2.20	1.20
7:A:3014:CLA:CHC	7:A:3029:CLA:C3D	2.21	1.17
7:A:3024:CLA:C3A	7:A:3027:CLA:CHD	2.39	1.00
1:A:45:UNK:CA	7:A:3071:CLA:C1A	2.38	1.00
2:B:343:UNK:CA	9:B:2008:SF4:S2	2.56	0.94
6:C:6:UNK:CA	6:C:68:UNK:CA	2.46	0.93
7:A:3024:CLA:C3A	7:A:3027:CLA:C4C	2.47	0.93
2:B:344:UNK:CA	9:B:2008:SF4:S1	2.57	0.92
7:A:3024:CLA:C2C	7:A:3030:CLA:C2A	2.48	0.91
7:A:3056:CLA:HHD	7:A:3057:CLA:C2A	2.01	0.91
1:A:362:UNK:CA	1:A:363:UNK:CA	2.50	0.90
2:B:428:UNK:CA	7:B:2005:CLA:C4A	2.50	0.89
1:A:45:UNK:CA	7:A:3071:CLA:CHA	2.51	0.88
7:A:3056:CLA:CHD	7:A:3057:CLA:C2A	2.51	0.87
1:A:44:UNK:CA	7:A:3071:CLA:C3D	2.55	0.85
1:A:326:UNK:CA	9:B:2008:SF4:S4	2.66	0.84
2:B:428:UNK:CA	7:B:2005:CLA:CHB	2.54	0.84
7:A:3007:CLA:C2C	7:F:3002:CLA:C3A	2.59	0.80
1:A:287:UNK:CA	1:A:288:UNK:CA	2.59	0.80
2:B:32:UNK:CA	7:B:3069:CLA:C2B	2.59	0.80
2:B:428:UNK:CA	7:B:2005:CLA:HHB	2.14	0.77
7:A:3027:CLA:C2A	7:A:3039:CLA:C2A	2.62	0.77
7:A:3014:CLA:C1C	7:A:3029:CLA:C3D	2.63	0.76
7:A:3056:CLA:C2D	7:A:3057:CLA:CHA	2.64	0.75
7:A:3007:CLA:CHC	7:F:3002:CLA:C2A	2.66	0.73
2:B:221:UNK:CA	2:B:222:UNK:CA	2.66	0.72
7:B:3001:CLA:C2D	7:F:3012:CLA:C2A	2.67	0.72
7:B:3001:CLA:C3D	7:F:3012:CLA:C2A	2.69	0.70
1:A:45:UNK:CA	7:A:3071:CLA:C2A	2.68	0.70
7:A:3016:CLA:C2A	7:A:3029:CLA:C3C	2.71	0.68
2:B:466:UNK:CA	2:B:467:UNK:CA	2.71	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:398:UNK:CA	1:A:460:UNK:CA	2.71	0.68
7:A:3014:CLA:C2C	7:A:3029:CLA:C3D	2.73	0.67
7:A:3014:CLA:HHC	7:A:3029:CLA:C2D	2.25	0.67
2:B:457:UNK:CA	2:B:458:UNK:CA	2.74	0.65
2:B:139:UNK:CA	2:B:140:UNK:CA	2.74	0.64
1:A:140:UNK:CA	1:A:141:UNK:CA	2.75	0.64
6:C:7:UNK:CA	6:C:68:UNK:CA	2.77	0.63
1:A:431:UNK:CA	1:A:432:UNK:CA	2.79	0.60
7:A:3016:CLA:C2A	7:A:3029:CLA:C2C	2.79	0.60
1:A:185:UNK:CA	7:A:3016:CLA:CHB	2.80	0.60
6:C:9:UNK:CA	6:C:67:UNK:CA	2.81	0.59
7:A:3005:CLA:C3B	7:A:3017:CLA:CHA	2.82	0.58
2:B:282:UNK:CA	7:B:3020:CLA:C2D	2.82	0.57
7:A:3024:CLA:C2A	7:A:3027:CLA:CHD	2.81	0.57
7:A:3024:CLA:HHB	7:A:3027:CLA:C3C	2.35	0.57
1:A:17:UNK:CA	7:A:3079:CLA:HHD	2.35	0.56
7:A:3024:CLA:C2A	7:A:3027:CLA:C1D	2.83	0.56
7:B:3003:CLA:C1B	7:B:3006:CLA:CHA	2.83	0.56
5:F:114:UNK:CA	7:F:3031:CLA:C2A	2.88	0.52
7:A:3014:CLA:C2C	7:A:3029:CLA:C2D	2.87	0.52
4:K:39:UNK:CA	4:K:40:UNK:CA	2.89	0.51
7:B:3003:CLA:C4B	7:B:3006:CLA:C2A	2.89	0.51
7:A:3005:CLA:C3A	7:A:3014:CLA:CHB	2.89	0.51
1:A:163:UNK:CA	7:A:3026:CLA:C3A	2.90	0.50
7:A:3024:CLA:CHB	7:A:3027:CLA:C3C	2.90	0.49
2:B:255:UNK:CA	2:B:256:UNK:CA	2.91	0.49
7:A:3016:CLA:C1A	7:A:3029:CLA:C3C	2.91	0.48
2:B:305:UNK:CA	2:B:306:UNK:CA	2.91	0.48
6:C:7:UNK:CA	6:C:8:UNK:CA	2.92	0.48
7:A:3005:CLA:C2A	7:A:3014:CLA:C3A	2.92	0.47
2:B:172:UNK:CA	2:B:173:UNK:CA	2.92	0.47
7:A:3016:CLA:C3A	7:A:3029:CLA:C3C	2.92	0.47
7:A:3024:CLA:C3A	7:A:3027:CLA:C1D	2.91	0.47
7:A:3027:CLA:C2A	7:A:3039:CLA:CHA	2.93	0.46
7:B:3011:CLA:C3D	7:B:3034:CLA:C2A	2.93	0.46
7:A:3027:CLA:C3A	7:A:3039:CLA:C2A	2.96	0.44
7:A:3007:CLA:C1C	7:F:3002:CLA:C2A	2.96	0.44
1:A:240:UNK:CA	1:A:241:UNK:CA	2.96	0.43
7:A:3007:CLA:HHC	7:F:3002:CLA:C2A	2.47	0.42
7:B:3011:CLA:C3D	7:B:3034:CLA:C3A	2.97	0.42
7:A:3007:CLA:HHC	7:F:3002:CLA:C1A	2.51	0.41
7:A:3018:CLA:C2D	7:A:3024:CLA:C2A	2.99	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:K:39:UNK:CA	4:K:41:UNK:CA	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 93 ligands modelled in this entry, 1 is modelled with single atom - leaving 92 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
7	CLA	A	2001	-	23,32,73	33.50	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	2006	-	23,32,73	33.38	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	2502	-	23,32,73	33.24	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3005	-	23,32,73	33.30	8 (34%)	12,54,113	2.27	4 (33%)
7	CLA	A	3007	-	23,32,73	33.39	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	A	3009	-	23,32,73	33.05	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3013	-	23,32,73	33.34	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	A	3014	-	23,32,73	33.20	8 (34%)	12,54,113	3.70	2 (16%)
7	CLA	A	3016	-	23,32,73	33.50	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	A	3017	-	23,32,73	33.40	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	A	3018	-	23,32,73	33.26	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	A	3021	-	23,32,73	33.26	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	A	3024	-	23,32,73	33.41	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3026	-	23,32,73	33.29	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3027	-	23,32,73	33.26	8 (34%)	12,54,113	2.31	4 (33%)
7	CLA	A	3029	-	23,32,73	33.41	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	A	3030	-	23,32,73	33.33	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3032	-	23,32,73	33.27	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3039	-	23,32,73	33.25	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3040	-	23,32,73	33.26	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3041	-	23,32,73	33.47	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3043	-	23,32,73	33.44	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3045	-	23,32,73	33.25	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3047	-	23,32,73	33.41	8 (34%)	12,54,113	2.27	4 (33%)
7	CLA	A	3048	-	23,32,73	33.58	8 (34%)	12,54,113	2.31	4 (33%)
7	CLA	A	3052	-	23,32,73	33.26	8 (34%)	12,54,113	2.27	4 (33%)
7	CLA	A	3053	-	23,32,73	33.31	8 (34%)	12,54,113	2.27	4 (33%)
7	CLA	A	3056	-	23,32,73	33.43	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3057	-	23,32,73	33.50	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	A	3058	-	23,32,73	33.44	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3062	-	23,32,73	33.52	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	A	3065	-	23,32,73	33.54	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3067	-	23,32,73	33.30	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	A	3068	-	23,32,73	33.17	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3071	-	23,32,73	33.44	8 (34%)	12,54,113	2.29	4 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CLA	A	3072	-	23,32,73	33.26	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	A	3073	-	23,32,73	33.22	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	A	3077	-	23,32,73	33.28	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	A	3078	-	23,32,73	33.26	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	A	3079	-	23,32,73	33.51	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	B	2002	-	23,32,73	33.12	8 (34%)	12,54,113	2.27	4 (33%)
7	CLA	B	2003	-	23,32,73	33.30	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	B	2004	-	23,32,73	33.13	8 (34%)	12,54,113	2.25	4 (33%)
7	CLA	B	2005	-	23,32,73	33.17	8 (34%)	12,54,113	2.29	4 (33%)
9	SF4	B	2008	-	12,12,12	18.71	12 (100%)	0,24,24	0.00	-
7	CLA	B	2501	-	23,32,73	33.38	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	B	3001	-	23,32,73	33.34	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	B	3003	-	23,32,73	33.48	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	B	3006	-	23,32,73	33.34	8 (34%)	12,54,113	2.31	4 (33%)
7	CLA	B	3008	-	23,32,73	33.19	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	B	3010	-	23,32,73	33.42	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	B	3011	-	23,32,73	33.43	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	B	3015	-	23,32,73	33.37	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	B	3019	-	23,32,73	33.36	8 (34%)	12,54,113	2.27	4 (33%)
7	CLA	B	3020	-	23,32,73	33.31	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	B	3023	-	23,32,73	33.40	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	B	3025	-	23,32,73	33.27	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	B	3028	-	23,32,73	33.44	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	B	3034	-	23,32,73	33.26	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	B	3035	-	23,32,73	33.24	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	B	3037	-	23,32,73	33.36	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	B	3042	-	23,32,73	33.31	8 (34%)	12,54,113	2.27	4 (33%)
7	CLA	B	3044	-	23,32,73	33.30	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	B	3046	-	23,32,73	33.27	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	B	3055	-	23,32,73	33.16	8 (34%)	12,54,113	2.27	4 (33%)
7	CLA	B	3060	-	23,32,73	33.48	8 (34%)	12,54,113	2.31	4 (33%)
7	CLA	B	3063	-	23,32,73	33.31	8 (34%)	12,54,113	2.27	4 (33%)
7	CLA	B	3066	-	23,32,73	33.29	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	B	3069	-	23,32,73	33.33	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	B	3070	-	23,32,73	33.30	8 (34%)	12,54,113	2.28	4 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CLA	B	3074	-	23,32,73	33.32	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	B	3075	-	23,32,73	33.26	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	B	3076	-	23,32,73	33.22	8 (34%)	12,54,113	2.27	4 (33%)
7	CLA	B	3080	-	23,32,73	33.37	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	B	3081	-	23,32,73	33.44	8 (34%)	12,54,113	2.29	4 (33%)
9	SF4	C	2009	-	12,12,12	18.71	12 (100%)	0,24,24	0.00	-
9	SF4	C	2010	-	12,12,12	25.87	9 (75%)	0,24,24	0.00	-
7	CLA	F	3002	-	23,32,73	33.49	8 (34%)	12,54,113	2.31	4 (33%)
7	CLA	F	3004	-	23,32,73	33.51	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	F	3012	-	23,32,73	33.23	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	F	3022	-	23,32,73	33.36	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	F	3031	-	23,32,73	32.93	8 (34%)	12,54,113	2.26	4 (33%)
7	CLA	F	3033	-	23,32,73	33.23	8 (34%)	12,54,113	2.29	4 (33%)
7	CLA	F	3054	-	23,32,73	33.41	8 (34%)	12,54,113	2.31	4 (33%)
7	CLA	F	3059	-	23,32,73	33.46	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	F	3061	-	23,32,73	33.42	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	K	3050	-	23,32,73	33.25	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	K	3051	-	23,32,73	33.17	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	L	3036	-	23,32,73	33.38	8 (34%)	12,54,113	2.30	4 (33%)
7	CLA	L	3038	-	23,32,73	33.00	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	L	3049	-	23,32,73	32.86	8 (34%)	12,54,113	2.28	4 (33%)
7	CLA	L	3064	-	23,32,73	33.25	8 (34%)	12,54,113	3.70	2 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLA	A	2001	-	-	0/0/66/135	0/0/8/9
7	CLA	A	2006	-	-	0/0/66/135	0/0/8/9
7	CLA	A	2502	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3005	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3007	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3009	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3013	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3014	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLA	A	3016	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3017	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3018	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3021	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3024	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3026	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3027	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3029	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3030	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3032	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3039	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3040	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3041	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3043	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3045	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3047	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3048	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3052	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3053	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3056	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3057	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3058	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3062	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3065	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3067	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3068	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3071	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3072	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3073	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3077	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3078	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3079	-	-	0/0/66/135	0/0/8/9
7	CLA	B	2002	-	-	0/0/66/135	0/0/8/9
7	CLA	B	2003	-	-	0/0/66/135	0/0/8/9
7	CLA	B	2004	-	-	0/0/66/135	0/0/8/9
7	CLA	B	2005	-	-	0/0/66/135	0/0/8/9
9	SF4	B	2008	-	-	0/0/48/48	0/6/5/5
7	CLA	B	2501	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3001	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3003	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3006	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3008	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLA	B	3010	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3011	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3015	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3019	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3020	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3023	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3025	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3028	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3034	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3035	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3037	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3042	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3044	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3046	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3055	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3060	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3063	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3066	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3069	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3070	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3074	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3075	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3076	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3080	-	-	0/0/66/135	0/0/8/9
7	CLA	B	3081	-	-	0/0/66/135	0/0/8/9
9	SF4	C	2009	-	-	0/0/48/48	0/6/5/5
9	SF4	C	2010	-	-	0/0/48/48	0/6/5/5
7	CLA	F	3002	-	-	0/0/66/135	0/0/8/9
7	CLA	F	3004	-	-	0/0/66/135	0/0/8/9
7	CLA	F	3012	-	-	0/0/66/135	0/0/8/9
7	CLA	F	3022	-	-	0/0/66/135	0/0/8/9
7	CLA	F	3031	-	-	0/0/66/135	0/0/8/9
7	CLA	F	3033	-	-	0/0/66/135	0/0/8/9
7	CLA	F	3054	-	-	0/0/66/135	0/0/8/9
7	CLA	F	3059	-	-	0/0/66/135	0/0/8/9
7	CLA	F	3061	-	-	0/0/66/135	0/0/8/9
7	CLA	K	3050	-	-	0/0/66/135	0/0/8/9
7	CLA	K	3051	-	-	0/0/66/135	0/0/8/9
7	CLA	L	3036	-	-	0/0/66/135	0/0/8/9
7	CLA	L	3038	-	-	0/0/66/135	0/0/8/9
7	CLA	L	3049	-	-	0/0/66/135	0/0/8/9
7	CLA	L	3064	-	-	0/0/66/135	0/0/8/9

All (745) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	3054	CLA	C3B-C4B	101.73	1.52	1.38
7	A	3048	CLA	C3B-C4B	101.72	1.52	1.38
7	B	3028	CLA	C3B-C4B	101.17	1.52	1.38
7	A	3065	CLA	C3B-C4B	101.15	1.52	1.38
7	A	2001	CLA	C3B-C4B	101.15	1.52	1.38
7	A	3057	CLA	C3B-C4B	101.10	1.52	1.38
7	B	3060	CLA	C3B-C4B	101.06	1.52	1.38
7	A	3079	CLA	C3B-C4B	101.04	1.52	1.38
7	A	3013	CLA	C3B-C4B	101.03	1.52	1.38
7	F	3002	CLA	C3B-C4B	101.01	1.52	1.38
7	A	3062	CLA	C3B-C4B	100.89	1.52	1.38
7	B	3011	CLA	C3B-C4B	100.84	1.52	1.38
7	B	3006	CLA	C3B-C4B	100.83	1.52	1.38
7	B	3037	CLA	C3B-C4B	100.80	1.52	1.38
7	B	3074	CLA	C3B-C4B	100.79	1.52	1.38
7	A	3072	CLA	C3B-C4B	100.78	1.52	1.38
7	A	3005	CLA	C3B-C4B	100.77	1.52	1.38
7	A	3056	CLA	C3B-C4B	100.77	1.52	1.38
7	F	3059	CLA	C3B-C4B	100.72	1.52	1.38
7	F	3061	CLA	C3B-C4B	100.71	1.52	1.38
7	B	3010	CLA	C3B-C4B	100.70	1.52	1.38
7	F	3022	CLA	C3B-C4B	100.67	1.52	1.38
7	A	3071	CLA	C3B-C4B	100.65	1.52	1.38
7	B	2004	CLA	C3B-C4B	100.60	1.52	1.38
7	A	3058	CLA	C3B-C4B	100.57	1.52	1.38
7	A	3073	CLA	C3B-C4B	100.57	1.52	1.38
7	A	3043	CLA	C3B-C4B	100.53	1.52	1.38
7	A	3021	CLA	C3B-C4B	100.53	1.52	1.38
7	A	3024	CLA	C3B-C4B	100.50	1.52	1.38
7	A	3007	CLA	C3B-C4B	100.50	1.52	1.38
7	B	3001	CLA	C3B-C4B	100.48	1.52	1.38
7	A	3014	CLA	C2D-C1D	100.46	1.52	1.38
7	B	3023	CLA	C3B-C4B	100.46	1.52	1.38
7	B	3081	CLA	C3B-C4B	100.44	1.52	1.38
7	B	2501	CLA	C3B-C4B	100.42	1.52	1.38
7	A	2502	CLA	C3B-C4B	100.42	1.52	1.38
7	B	3019	CLA	C3B-C4B	100.40	1.52	1.38
7	L	3038	CLA	C3B-C4B	100.35	1.52	1.38
7	A	3016	CLA	C3B-C4B	100.34	1.52	1.38
7	B	3020	CLA	C3B-C4B	100.33	1.52	1.38
7	A	3017	CLA	C3B-C4B	100.32	1.52	1.38
7	A	3053	CLA	C3B-C4B	100.29	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	3004	CLA	C3B-C4B	100.26	1.52	1.38
7	A	3077	CLA	C3B-C4B	100.25	1.52	1.38
7	B	3015	CLA	C3B-C4B	100.25	1.52	1.38
7	L	3064	CLA	C2D-C1D	100.24	1.52	1.38
7	B	3066	CLA	C3B-C4B	100.22	1.52	1.38
7	K	3050	CLA	C3B-C4B	100.22	1.52	1.38
7	A	3067	CLA	C3B-C4B	100.19	1.52	1.38
7	A	3039	CLA	C3B-C4B	100.18	1.52	1.38
7	A	3045	CLA	C3B-C4B	100.16	1.52	1.38
7	A	3052	CLA	C3B-C4B	100.15	1.52	1.38
7	A	3041	CLA	C3B-C4B	100.15	1.52	1.38
7	A	3068	CLA	C3B-C4B	100.14	1.52	1.38
7	B	2003	CLA	C3B-C4B	100.13	1.52	1.38
7	F	3033	CLA	C3B-C4B	100.12	1.52	1.38
7	B	3008	CLA	C3B-C4B	100.08	1.52	1.38
7	B	3044	CLA	C3B-C4B	100.07	1.52	1.38
7	B	3075	CLA	C3B-C4B	100.07	1.52	1.38
7	A	3078	CLA	C3B-C4B	100.06	1.52	1.38
7	B	2005	CLA	C3B-C4B	100.06	1.52	1.38
7	L	3036	CLA	C3B-C4B	100.04	1.52	1.38
7	B	3076	CLA	C3B-C4B	99.96	1.52	1.38
7	B	3003	CLA	C3B-C4B	99.96	1.52	1.38
7	B	3069	CLA	C3B-C4B	99.95	1.52	1.38
7	A	3032	CLA	C3B-C4B	99.93	1.52	1.38
7	B	3042	CLA	C3B-C4B	99.93	1.52	1.38
7	A	3026	CLA	C3B-C4B	99.91	1.52	1.38
7	F	3012	CLA	C3B-C4B	99.90	1.52	1.38
7	A	3029	CLA	C3B-C4B	99.85	1.52	1.38
7	B	3046	CLA	C3B-C4B	99.84	1.52	1.38
7	B	3070	CLA	C3B-C4B	99.83	1.52	1.38
7	B	3025	CLA	C3B-C4B	99.81	1.52	1.38
7	A	3027	CLA	C3B-C4B	99.77	1.52	1.38
7	A	3030	CLA	C3B-C4B	99.73	1.52	1.38
7	A	3040	CLA	C3B-C4B	99.71	1.52	1.38
7	B	3055	CLA	C3B-C4B	99.71	1.52	1.38
7	A	2006	CLA	C3B-C4B	99.67	1.52	1.38
7	B	3080	CLA	C3B-C4B	99.64	1.52	1.38
7	B	3034	CLA	C3B-C4B	99.64	1.52	1.38
7	B	3063	CLA	C3B-C4B	99.61	1.52	1.38
7	K	3051	CLA	C3B-C4B	99.56	1.52	1.38
7	B	3035	CLA	C3B-C4B	99.50	1.52	1.38
7	A	3018	CLA	C3B-C4B	99.49	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	3031	CLA	C3B-C4B	99.36	1.52	1.38
7	A	3047	CLA	C3B-C4B	99.13	1.52	1.38
7	B	2002	CLA	C3B-C4B	98.86	1.52	1.38
7	A	3009	CLA	C3B-C4B	98.56	1.52	1.38
7	L	3049	CLA	C3B-C4B	98.52	1.52	1.38
7	A	2006	CLA	C2B-C1B	93.95	1.51	1.38
7	F	3002	CLA	C2B-C1B	93.82	1.51	1.38
7	B	3003	CLA	C2B-C1B	93.76	1.51	1.38
7	B	3060	CLA	C2B-C1B	93.73	1.51	1.38
7	A	3043	CLA	C2B-C1B	93.67	1.51	1.38
7	B	3010	CLA	C2B-C1B	93.52	1.51	1.38
7	A	3030	CLA	C2B-C1B	93.50	1.51	1.38
7	A	3071	CLA	C2B-C1B	93.47	1.51	1.38
7	A	3016	CLA	C2B-C1B	93.42	1.51	1.38
7	F	3004	CLA	C2B-C1B	93.41	1.51	1.38
7	B	3080	CLA	C2B-C1B	93.41	1.51	1.38
7	B	3070	CLA	C2B-C1B	93.40	1.51	1.38
7	B	3081	CLA	C2B-C1B	93.39	1.51	1.38
7	B	2501	CLA	C2B-C1B	93.39	1.51	1.38
7	A	3041	CLA	C2B-C1B	93.38	1.51	1.38
7	B	3015	CLA	C2B-C1B	93.33	1.51	1.38
7	A	3062	CLA	C2B-C1B	93.32	1.51	1.38
7	A	3048	CLA	C2B-C1B	93.27	1.51	1.38
7	A	3053	CLA	C2B-C1B	93.24	1.51	1.38
7	B	3028	CLA	C2B-C1B	93.21	1.51	1.38
7	A	3027	CLA	C2B-C1B	93.19	1.51	1.38
7	F	3033	CLA	C2B-C1B	93.17	1.51	1.38
7	F	3061	CLA	C2B-C1B	93.16	1.51	1.38
7	L	3036	CLA	C2B-C1B	93.15	1.51	1.38
7	A	3065	CLA	C2B-C1B	93.11	1.51	1.38
7	B	2003	CLA	C2B-C1B	93.10	1.51	1.38
7	A	3079	CLA	C2B-C1B	93.10	1.51	1.38
7	A	3047	CLA	C2B-C1B	93.10	1.51	1.38
7	B	3034	CLA	C2B-C1B	93.10	1.51	1.38
7	A	3018	CLA	C2B-C1B	93.10	1.51	1.38
7	B	3063	CLA	C2B-C1B	93.10	1.51	1.38
7	B	3011	CLA	C2B-C1B	93.09	1.51	1.38
7	F	3059	CLA	C2B-C1B	93.09	1.51	1.38
7	A	3056	CLA	C2B-C1B	93.07	1.51	1.38
7	A	3072	CLA	C2B-C1B	93.07	1.51	1.38
7	A	3017	CLA	C2B-C1B	93.06	1.51	1.38
7	A	3026	CLA	C2B-C1B	93.04	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3001	CLA	C2B-C1B	93.03	1.51	1.38
7	B	3042	CLA	C2B-C1B	93.03	1.51	1.38
7	A	3057	CLA	C2B-C1B	93.02	1.51	1.38
7	A	3039	CLA	C2B-C1B	93.01	1.51	1.38
7	B	3046	CLA	C2B-C1B	92.98	1.51	1.38
7	A	3058	CLA	C2B-C1B	92.94	1.51	1.38
7	A	3007	CLA	C2B-C1B	92.91	1.51	1.38
7	B	3074	CLA	C2B-C1B	92.90	1.51	1.38
7	B	3023	CLA	C2B-C1B	92.89	1.51	1.38
7	B	3069	CLA	C2B-C1B	92.87	1.51	1.38
7	B	3035	CLA	C2B-C1B	92.86	1.51	1.38
7	B	3019	CLA	C2B-C1B	92.86	1.51	1.38
7	A	3073	CLA	C2B-C1B	92.85	1.51	1.38
7	F	3054	CLA	C2B-C1B	92.84	1.51	1.38
7	A	2001	CLA	C2B-C1B	92.82	1.51	1.38
7	L	3064	CLA	C3D-C4D	92.79	1.51	1.38
7	A	3024	CLA	C2B-C1B	92.78	1.51	1.38
7	B	3025	CLA	C2B-C1B	92.75	1.51	1.38
7	B	2005	CLA	C2B-C1B	92.75	1.51	1.38
7	A	3029	CLA	C2B-C1B	92.73	1.51	1.38
7	A	3032	CLA	C2B-C1B	92.73	1.51	1.38
7	F	3022	CLA	C2B-C1B	92.72	1.51	1.38
7	B	3020	CLA	C2B-C1B	92.71	1.51	1.38
7	A	3014	CLA	C3D-C4D	92.66	1.51	1.38
7	A	3067	CLA	C2B-C1B	92.66	1.51	1.38
7	B	2002	CLA	C2B-C1B	92.64	1.51	1.38
7	A	3040	CLA	C2B-C1B	92.64	1.51	1.38
7	A	3068	CLA	C2B-C1B	92.64	1.51	1.38
7	B	3037	CLA	C2B-C1B	92.61	1.51	1.38
7	A	2502	CLA	C2B-C1B	92.58	1.51	1.38
7	A	3045	CLA	C2B-C1B	92.54	1.51	1.38
7	B	3055	CLA	C2B-C1B	92.53	1.51	1.38
7	A	3077	CLA	C2B-C1B	92.51	1.51	1.38
7	B	3006	CLA	C2B-C1B	92.50	1.51	1.38
7	A	3078	CLA	C2B-C1B	92.49	1.51	1.38
7	B	3076	CLA	C2B-C1B	92.46	1.51	1.38
7	A	3052	CLA	C2B-C1B	92.46	1.51	1.38
7	F	3012	CLA	C2B-C1B	92.46	1.51	1.38
7	A	3021	CLA	C2B-C1B	92.46	1.51	1.38
7	K	3051	CLA	C2B-C1B	92.42	1.51	1.38
7	K	3050	CLA	C2B-C1B	92.41	1.51	1.38
7	B	3044	CLA	C2B-C1B	92.38	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3005	CLA	C2B-C1B	92.35	1.51	1.38
7	B	3066	CLA	C2B-C1B	92.35	1.51	1.38
7	A	3009	CLA	C2B-C1B	92.23	1.51	1.38
7	B	3075	CLA	C2B-C1B	91.94	1.51	1.38
7	A	3013	CLA	C2B-C1B	91.88	1.51	1.38
7	F	3031	CLA	C2B-C1B	91.77	1.51	1.38
7	L	3049	CLA	C2B-C1B	91.71	1.51	1.38
7	B	3008	CLA	C2B-C1B	91.53	1.51	1.38
7	B	2004	CLA	C2B-C1B	91.26	1.51	1.38
7	L	3038	CLA	C2B-C1B	91.19	1.51	1.38
7	A	3016	CLA	C3D-C4D	63.10	1.47	1.38
7	B	3003	CLA	C3D-C4D	62.79	1.47	1.38
7	L	3036	CLA	C3D-C4D	62.78	1.47	1.38
7	B	3008	CLA	C3D-C4D	62.72	1.47	1.38
7	B	2002	CLA	C3D-C4D	62.65	1.47	1.38
7	A	3065	CLA	C3D-C4D	62.61	1.47	1.38
7	F	3004	CLA	C3D-C4D	62.59	1.47	1.38
7	B	3069	CLA	C3D-C4D	62.55	1.47	1.38
7	A	3017	CLA	C3D-C4D	62.50	1.47	1.38
7	A	3079	CLA	C3D-C4D	62.48	1.47	1.38
7	B	3066	CLA	C3D-C4D	62.45	1.47	1.38
7	B	3034	CLA	C3D-C4D	62.41	1.47	1.38
7	A	3067	CLA	C3D-C4D	62.40	1.47	1.38
7	A	3041	CLA	C3D-C4D	62.38	1.47	1.38
7	A	3048	CLA	C3D-C4D	62.38	1.47	1.38
7	A	3047	CLA	C3D-C4D	62.38	1.47	1.38
7	A	3024	CLA	C3D-C4D	62.35	1.47	1.38
7	A	3062	CLA	C3D-C4D	62.35	1.47	1.38
7	A	3078	CLA	C3D-C4D	62.33	1.47	1.38
7	A	3029	CLA	C3D-C4D	62.30	1.47	1.38
7	B	3042	CLA	C3D-C4D	62.29	1.47	1.38
7	B	3063	CLA	C3D-C4D	62.28	1.47	1.38
7	F	3059	CLA	C3D-C4D	62.25	1.47	1.38
7	A	3071	CLA	C3D-C4D	62.23	1.47	1.38
7	A	3026	CLA	C3D-C4D	62.21	1.47	1.38
7	A	3009	CLA	C3D-C4D	62.20	1.47	1.38
7	A	3058	CLA	C3D-C4D	62.19	1.47	1.38
7	B	3044	CLA	C3D-C4D	62.12	1.47	1.38
7	A	3056	CLA	C3D-C4D	62.10	1.47	1.38
7	A	3040	CLA	C3D-C4D	62.09	1.47	1.38
7	B	3055	CLA	C3D-C4D	62.05	1.47	1.38
7	K	3051	CLA	C3D-C4D	62.03	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3035	CLA	C3D-C4D	61.99	1.47	1.38
7	B	2501	CLA	C3D-C4D	61.99	1.47	1.38
7	A	2001	CLA	C3D-C4D	61.99	1.47	1.38
7	B	3025	CLA	C3D-C4D	61.98	1.47	1.38
7	A	3030	CLA	C3D-C4D	61.97	1.47	1.38
7	A	3077	CLA	C3D-C4D	61.97	1.47	1.38
7	B	3075	CLA	C3D-C4D	61.95	1.47	1.38
7	B	3015	CLA	C3D-C4D	61.95	1.47	1.38
7	A	3052	CLA	C3D-C4D	61.94	1.47	1.38
7	B	3080	CLA	C3D-C4D	61.93	1.47	1.38
7	L	3064	CLA	C2B-C1B	61.92	1.47	1.38
7	F	3022	CLA	C3D-C4D	61.89	1.47	1.38
7	B	3081	CLA	C3D-C4D	61.86	1.47	1.38
7	B	3060	CLA	C3D-C4D	61.83	1.47	1.38
7	B	3006	CLA	C3D-C4D	61.83	1.47	1.38
7	L	3049	CLA	C3D-C4D	61.83	1.47	1.38
7	B	3070	CLA	C3D-C4D	61.82	1.47	1.38
7	A	3043	CLA	C3D-C4D	61.80	1.47	1.38
7	A	3018	CLA	C3D-C4D	61.79	1.47	1.38
7	A	3007	CLA	C3D-C4D	61.79	1.47	1.38
7	B	3011	CLA	C3D-C4D	61.77	1.47	1.38
7	B	3010	CLA	C3D-C4D	61.75	1.47	1.38
7	K	3050	CLA	C3D-C4D	61.74	1.47	1.38
7	A	3045	CLA	C3D-C4D	61.73	1.47	1.38
7	B	3023	CLA	C3D-C4D	61.71	1.47	1.38
7	F	3012	CLA	C3D-C4D	61.71	1.47	1.38
7	B	3046	CLA	C3D-C4D	61.69	1.47	1.38
7	F	3033	CLA	C3D-C4D	61.69	1.47	1.38
7	F	3061	CLA	C3D-C4D	61.68	1.47	1.38
7	A	3021	CLA	C3D-C4D	61.67	1.47	1.38
7	B	3001	CLA	C3D-C4D	61.62	1.47	1.38
7	A	3014	CLA	C2B-C1B	61.60	1.47	1.38
7	B	2004	CLA	C3D-C4D	61.56	1.47	1.38
7	B	3076	CLA	C3D-C4D	61.54	1.47	1.38
7	A	3057	CLA	C3D-C4D	61.54	1.47	1.38
7	A	3032	CLA	C3D-C4D	61.53	1.47	1.38
7	A	3027	CLA	C3D-C4D	61.52	1.47	1.38
7	B	3020	CLA	C3D-C4D	61.49	1.47	1.38
7	B	3037	CLA	C3D-C4D	61.49	1.47	1.38
7	A	3053	CLA	C3D-C4D	61.47	1.47	1.38
7	A	3039	CLA	C3D-C4D	61.45	1.47	1.38
7	A	3013	CLA	C3D-C4D	61.45	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2502	CLA	C3D-C4D	61.37	1.47	1.38
7	F	3031	CLA	C3D-C4D	61.36	1.47	1.38
7	B	3074	CLA	C3D-C4D	61.34	1.47	1.38
7	A	3005	CLA	C3D-C4D	61.32	1.47	1.38
7	B	3019	CLA	C3D-C4D	61.28	1.47	1.38
7	A	2006	CLA	C3D-C4D	61.27	1.47	1.38
7	B	3028	CLA	C3D-C4D	61.23	1.47	1.38
7	A	3068	CLA	C3D-C4D	61.18	1.47	1.38
7	F	3002	CLA	C3D-C4D	61.17	1.47	1.38
7	L	3038	CLA	C3D-C4D	61.05	1.47	1.38
7	A	3073	CLA	C3D-C4D	60.92	1.47	1.38
7	A	3072	CLA	C3D-C4D	60.83	1.47	1.38
7	B	2003	CLA	C3D-C4D	60.77	1.47	1.38
7	B	2005	CLA	C3D-C4D	60.72	1.47	1.38
7	F	3054	CLA	C3D-C4D	60.67	1.47	1.38
7	A	3047	CLA	C2D-C1D	54.29	1.46	1.38
7	A	3029	CLA	C2D-C1D	53.78	1.46	1.38
7	B	3019	CLA	C2D-C1D	53.07	1.46	1.38
7	A	3013	CLA	C2D-C1D	52.99	1.46	1.38
7	A	3057	CLA	C2D-C1D	52.95	1.45	1.38
7	B	3075	CLA	C2D-C1D	52.92	1.45	1.38
7	F	3004	CLA	C2D-C1D	52.92	1.45	1.38
7	B	3080	CLA	C2D-C1D	52.89	1.45	1.38
7	A	3041	CLA	C2D-C1D	52.83	1.45	1.38
7	B	3023	CLA	C2D-C1D	52.80	1.45	1.38
7	A	2006	CLA	C2D-C1D	52.70	1.45	1.38
7	B	2003	CLA	C2D-C1D	52.69	1.45	1.38
9	C	2010	SF4	S3-FE1	-52.61	1.97	2.33
7	A	3058	CLA	C2D-C1D	52.55	1.45	1.38
7	B	3044	CLA	C2D-C1D	52.54	1.45	1.38
7	A	3007	CLA	C2D-C1D	52.50	1.45	1.38
7	A	2001	CLA	C2D-C1D	52.47	1.45	1.38
7	A	3032	CLA	C2D-C1D	52.47	1.45	1.38
7	A	3024	CLA	C2D-C1D	52.40	1.45	1.38
7	B	3081	CLA	C2D-C1D	52.33	1.45	1.38
7	A	3062	CLA	C2D-C1D	52.32	1.45	1.38
7	B	3020	CLA	C2D-C1D	52.31	1.45	1.38
7	F	3059	CLA	C2D-C1D	52.30	1.45	1.38
7	B	3037	CLA	C2D-C1D	52.23	1.45	1.38
7	A	3005	CLA	C2D-C1D	52.22	1.45	1.38
7	B	3003	CLA	C2D-C1D	52.22	1.45	1.38
7	F	3012	CLA	C2D-C1D	52.21	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3040	CLA	C2D-C1D	52.20	1.45	1.38
7	A	3018	CLA	C2D-C1D	52.17	1.45	1.38
7	B	3035	CLA	C2D-C1D	52.17	1.45	1.38
7	B	3076	CLA	C2D-C1D	52.14	1.45	1.38
7	F	3002	CLA	C2D-C1D	52.13	1.45	1.38
7	B	3025	CLA	C2D-C1D	52.11	1.45	1.38
7	B	3011	CLA	C2D-C1D	52.11	1.45	1.38
7	F	3061	CLA	C2D-C1D	52.11	1.45	1.38
7	L	3064	CLA	C3B-C4B	52.08	1.45	1.38
7	A	3065	CLA	C2D-C1D	52.07	1.45	1.38
7	B	3028	CLA	C2D-C1D	52.06	1.45	1.38
7	A	3079	CLA	C2D-C1D	52.05	1.45	1.38
7	B	3063	CLA	C2D-C1D	52.05	1.45	1.38
7	A	3009	CLA	C2D-C1D	52.02	1.45	1.38
7	A	3016	CLA	C2D-C1D	51.99	1.45	1.38
7	K	3050	CLA	C2D-C1D	51.98	1.45	1.38
7	F	3022	CLA	C2D-C1D	51.97	1.45	1.38
7	B	3046	CLA	C2D-C1D	51.97	1.45	1.38
7	A	3056	CLA	C2D-C1D	51.89	1.45	1.38
7	A	3017	CLA	C2D-C1D	51.89	1.45	1.38
7	B	3006	CLA	C2D-C1D	51.88	1.45	1.38
7	A	3045	CLA	C2D-C1D	51.87	1.45	1.38
7	A	3027	CLA	C2D-C1D	51.85	1.45	1.38
7	A	3030	CLA	C2D-C1D	51.83	1.45	1.38
7	F	3054	CLA	C2D-C1D	51.83	1.45	1.38
7	B	3069	CLA	C2D-C1D	51.81	1.45	1.38
7	A	3077	CLA	C2D-C1D	51.79	1.45	1.38
7	B	3001	CLA	C2D-C1D	51.79	1.45	1.38
7	A	3043	CLA	C2D-C1D	51.79	1.45	1.38
7	A	3052	CLA	C2D-C1D	51.74	1.45	1.38
7	B	3015	CLA	C2D-C1D	51.73	1.45	1.38
7	B	3066	CLA	C2D-C1D	51.73	1.45	1.38
7	B	3008	CLA	C2D-C1D	51.71	1.45	1.38
7	K	3051	CLA	C2D-C1D	51.70	1.45	1.38
7	B	2005	CLA	C2D-C1D	51.69	1.45	1.38
7	B	3042	CLA	C2D-C1D	51.68	1.45	1.38
7	A	3048	CLA	C2D-C1D	51.62	1.45	1.38
7	A	3078	CLA	C2D-C1D	51.62	1.45	1.38
7	A	2502	CLA	C2D-C1D	51.59	1.45	1.38
7	A	3021	CLA	C2D-C1D	51.58	1.45	1.38
7	L	3036	CLA	C2D-C1D	51.56	1.45	1.38
7	A	3071	CLA	C2D-C1D	51.53	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3053	CLA	C2D-C1D	51.52	1.45	1.38
7	B	3074	CLA	C2D-C1D	51.47	1.45	1.38
7	A	3014	CLA	C3B-C4B	51.45	1.45	1.38
7	A	3026	CLA	C2D-C1D	51.45	1.45	1.38
7	B	3070	CLA	C2D-C1D	51.45	1.45	1.38
7	A	3067	CLA	C2D-C1D	51.45	1.45	1.38
7	B	2004	CLA	C2D-C1D	51.39	1.45	1.38
7	B	3010	CLA	C2D-C1D	51.37	1.45	1.38
7	B	2501	CLA	C2D-C1D	51.29	1.45	1.38
7	B	3034	CLA	C2D-C1D	51.27	1.45	1.38
7	B	3060	CLA	C2D-C1D	51.26	1.45	1.38
7	A	3039	CLA	C2D-C1D	51.23	1.45	1.38
7	B	2002	CLA	C2D-C1D	51.09	1.45	1.38
7	A	3068	CLA	C2D-C1D	51.09	1.45	1.38
7	A	3073	CLA	C2D-C1D	51.02	1.45	1.38
7	B	3055	CLA	C2D-C1D	50.97	1.45	1.38
7	A	3072	CLA	C2D-C1D	50.90	1.45	1.38
7	L	3038	CLA	C2D-C1D	50.87	1.45	1.38
7	L	3049	CLA	C2D-C1D	50.58	1.45	1.38
7	F	3033	CLA	C2D-C1D	50.48	1.45	1.38
7	F	3031	CLA	C2D-C1D	50.41	1.45	1.38
9	C	2010	SF4	S2-FE4	-46.53	2.02	2.33
9	C	2010	SF4	S3-FE2	-37.52	2.08	2.33
9	C	2009	SF4	S2-FE3	-34.88	2.09	2.33
9	B	2008	SF4	S2-FE3	-34.87	2.09	2.33
9	C	2010	SF4	S4-FE3	-32.18	2.11	2.33
9	C	2009	SF4	S3-FE4	-31.14	2.12	2.33
9	B	2008	SF4	S3-FE4	-31.13	2.12	2.33
9	B	2008	SF4	S2-FE4	-23.50	2.17	2.33
9	C	2009	SF4	S2-FE4	-23.45	2.17	2.33
9	B	2008	SF4	S2-FE1	-21.15	2.19	2.33
9	C	2009	SF4	S2-FE1	-21.04	2.19	2.33
9	C	2009	SF4	S4-FE2	-20.06	2.19	2.33
9	B	2008	SF4	S4-FE2	-20.00	2.19	2.33
7	A	2001	CLA	C2A-C1A	16.99	1.47	1.39
7	B	2004	CLA	C2A-C1A	16.90	1.47	1.39
7	B	3063	CLA	C2A-C1A	16.82	1.47	1.39
7	B	3037	CLA	C2A-C1A	16.76	1.47	1.39
7	L	3038	CLA	C2A-C1A	16.74	1.47	1.39
7	A	3057	CLA	C2A-C1A	16.69	1.47	1.39
7	B	3010	CLA	C2A-C1A	16.68	1.47	1.39
7	F	3054	CLA	C2A-C1A	16.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3052	CLA	C2A-C1A	16.62	1.47	1.39
7	F	3031	CLA	C2A-C1A	16.61	1.47	1.39
7	B	3020	CLA	C2A-C1A	16.60	1.47	1.39
7	A	3053	CLA	C2A-C1A	16.59	1.47	1.39
7	F	3061	CLA	C2A-C1A	16.57	1.47	1.39
7	B	2501	CLA	C2A-C1A	16.57	1.47	1.39
7	B	3070	CLA	C2A-C1A	16.56	1.47	1.39
7	B	3076	CLA	C2A-C1A	16.56	1.47	1.39
7	B	3023	CLA	C2A-C1A	16.54	1.47	1.39
7	A	3058	CLA	C2A-C1A	16.53	1.47	1.39
7	B	3025	CLA	C2A-C1A	16.52	1.47	1.39
7	A	3056	CLA	C2A-C1A	16.52	1.47	1.39
7	B	3075	CLA	C2A-C1A	16.51	1.47	1.39
7	A	3007	CLA	C2A-C1A	16.50	1.47	1.39
7	F	3004	CLA	C2A-C1A	16.50	1.47	1.39
7	B	3008	CLA	C2A-C1A	16.50	1.47	1.39
7	K	3050	CLA	C2A-C1A	16.50	1.47	1.39
7	B	3015	CLA	C2A-C1A	16.49	1.47	1.39
7	F	3002	CLA	C2A-C1A	16.48	1.47	1.39
7	A	3068	CLA	C2A-C1A	16.48	1.47	1.39
7	B	3069	CLA	C2A-C1A	16.48	1.47	1.39
7	A	3024	CLA	C2A-C1A	16.48	1.47	1.39
7	B	3081	CLA	C2A-C1A	16.48	1.47	1.39
7	K	3051	CLA	C2A-C1A	16.47	1.47	1.39
7	A	3045	CLA	C2A-C1A	16.47	1.47	1.39
7	A	3067	CLA	C2A-C1A	16.47	1.47	1.39
7	L	3049	CLA	C2A-C1A	16.46	1.47	1.39
7	L	3036	CLA	C2A-C1A	16.46	1.47	1.39
7	A	3013	CLA	C2A-C1A	16.46	1.47	1.39
7	A	3005	CLA	C2A-C1A	16.45	1.47	1.39
7	B	3011	CLA	C2A-C1A	16.45	1.47	1.39
7	A	3077	CLA	C2A-C1A	16.44	1.47	1.39
7	B	3074	CLA	C2A-C1A	16.44	1.47	1.39
7	A	3072	CLA	C2A-C1A	16.44	1.47	1.39
7	A	3040	CLA	C2A-C1A	16.44	1.47	1.39
7	A	2006	CLA	C2A-C1A	16.43	1.47	1.39
7	A	3032	CLA	C2A-C1A	16.43	1.47	1.39
7	A	3047	CLA	C2A-C1A	16.43	1.47	1.39
7	B	3055	CLA	C2A-C1A	16.43	1.47	1.39
7	A	3065	CLA	C2A-C1A	16.42	1.47	1.39
7	B	3046	CLA	C2A-C1A	16.42	1.47	1.39
7	A	3016	CLA	C2A-C1A	16.41	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2005	CLA	C2A-C1A	16.40	1.47	1.39
7	A	3029	CLA	C2A-C1A	16.40	1.47	1.39
7	F	3012	CLA	C2A-C1A	16.40	1.47	1.39
7	A	3073	CLA	C2A-C1A	16.39	1.47	1.39
7	A	3078	CLA	C2A-C1A	16.39	1.47	1.39
7	A	3039	CLA	C2A-C1A	16.37	1.47	1.39
7	B	2002	CLA	C2A-C1A	16.36	1.47	1.39
7	B	3006	CLA	C2A-C1A	16.36	1.47	1.39
7	B	3044	CLA	C2A-C1A	16.35	1.47	1.39
7	A	3043	CLA	C2A-C1A	16.35	1.47	1.39
7	A	3009	CLA	C2A-C1A	16.35	1.47	1.39
7	F	3022	CLA	C2A-C1A	16.35	1.47	1.39
7	A	3026	CLA	C2A-C1A	16.34	1.47	1.39
7	B	3066	CLA	C2A-C1A	16.34	1.47	1.39
7	F	3059	CLA	C2A-C1A	16.33	1.47	1.39
7	A	3062	CLA	C2A-C1A	16.33	1.47	1.39
7	B	3060	CLA	C2A-C1A	16.32	1.47	1.39
7	A	3017	CLA	C2A-C1A	16.32	1.47	1.39
7	B	3001	CLA	C2A-C1A	16.32	1.47	1.39
7	A	3021	CLA	C2A-C1A	16.31	1.47	1.39
7	A	3018	CLA	C2A-C1A	16.30	1.47	1.39
7	A	2502	CLA	C2A-C1A	16.30	1.47	1.39
7	A	3079	CLA	C2A-C1A	16.29	1.47	1.39
7	A	3048	CLA	C2A-C1A	16.28	1.47	1.39
7	F	3033	CLA	C2A-C1A	16.28	1.47	1.39
7	A	3030	CLA	C2A-C1A	16.28	1.47	1.39
7	B	3003	CLA	C2A-C1A	16.27	1.47	1.39
7	A	3071	CLA	C2A-C1A	16.26	1.47	1.39
7	A	3041	CLA	C2A-C1A	16.26	1.47	1.39
7	B	3080	CLA	C2A-C1A	16.25	1.47	1.39
7	B	3042	CLA	C2A-C1A	16.25	1.47	1.39
7	B	3035	CLA	C2A-C1A	16.22	1.47	1.39
7	B	3019	CLA	C2A-C1A	16.22	1.47	1.39
7	B	3028	CLA	C2A-C1A	16.21	1.47	1.39
9	C	2010	SF4	S2-FE1	16.19	2.44	2.33
7	B	3034	CLA	C2A-C1A	16.15	1.47	1.39
7	A	3027	CLA	C2A-C1A	16.11	1.47	1.39
7	B	2003	CLA	C2A-C1A	15.96	1.47	1.39
9	B	2008	SF4	S4-FE3	-13.84	2.23	2.33
9	C	2009	SF4	S4-FE3	-13.77	2.24	2.33
7	A	3014	CLA	C2A-C1A	13.55	1.46	1.39
7	L	3064	CLA	C2A-C1A	13.26	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2008	SF4	S1-FE2	-12.57	2.24	2.33
9	C	2009	SF4	S1-FE2	-12.51	2.24	2.33
9	C	2010	SF4	S2-FE3	-11.42	2.25	2.33
9	B	2008	SF4	S4-FE1	10.63	2.40	2.33
9	C	2009	SF4	S4-FE1	10.63	2.40	2.33
9	C	2010	SF4	S1-FE4	-9.86	2.26	2.33
9	C	2010	SF4	S1-FE3	-9.69	2.26	2.33
9	C	2010	SF4	S4-FE1	-8.18	2.27	2.33
9	C	2009	SF4	S1-FE4	-7.67	2.28	2.33
9	B	2008	SF4	S1-FE4	-7.56	2.28	2.33
9	B	2008	SF4	S1-FE3	7.00	2.38	2.33
9	C	2009	SF4	S1-FE3	7.00	2.38	2.33
7	B	2003	CLA	MG-NB	6.67	2.19	2.05
7	A	2001	CLA	MG-NB	6.47	2.19	2.05
7	F	3061	CLA	MG-NB	6.23	2.18	2.05
7	A	3068	CLA	MG-NB	6.23	2.18	2.05
7	B	2501	CLA	MG-NB	6.21	2.18	2.05
7	A	3048	CLA	MG-NB	6.20	2.18	2.05
7	B	3010	CLA	MG-NB	6.20	2.18	2.05
7	B	3063	CLA	MG-NB	6.19	2.18	2.05
7	B	3020	CLA	MG-NB	6.19	2.18	2.05
7	B	3003	CLA	MG-NB	6.19	2.18	2.05
7	A	3029	CLA	MG-NB	6.19	2.18	2.05
7	A	3058	CLA	MG-NB	6.18	2.18	2.05
7	A	3026	CLA	MG-NB	6.18	2.18	2.05
7	A	3073	CLA	MG-NB	6.17	2.18	2.05
7	B	3028	CLA	MG-NB	6.17	2.18	2.05
7	B	3070	CLA	MG-NB	6.17	2.18	2.05
7	B	3060	CLA	MG-NB	6.17	2.18	2.05
7	A	3021	CLA	MG-NB	6.17	2.18	2.05
7	A	3047	CLA	MG-NB	6.16	2.18	2.05
7	F	3022	CLA	MG-NB	6.17	2.18	2.05
7	B	3001	CLA	MG-NB	6.16	2.18	2.05
7	B	3006	CLA	MG-NB	6.16	2.18	2.05
7	A	3072	CLA	MG-NB	6.15	2.18	2.05
7	A	3016	CLA	MG-NB	6.15	2.18	2.05
7	A	3040	CLA	MG-NB	6.15	2.18	2.05
7	A	3056	CLA	MG-NB	6.15	2.18	2.05
7	A	3039	CLA	MG-NB	6.15	2.18	2.05
7	A	3053	CLA	MG-NB	6.15	2.18	2.05
7	B	3046	CLA	MG-NB	6.15	2.18	2.05
7	A	3014	CLA	MG-ND	6.15	2.18	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3069	CLA	MG-NB	6.15	2.18	2.05
7	A	3077	CLA	MG-NB	6.15	2.18	2.05
7	A	3043	CLA	MG-NB	6.15	2.18	2.05
7	B	3066	CLA	MG-NB	6.15	2.18	2.05
7	B	3015	CLA	MG-NB	6.14	2.18	2.05
7	A	3007	CLA	MG-NB	6.14	2.18	2.05
7	B	3074	CLA	MG-NB	6.14	2.18	2.05
7	B	3034	CLA	MG-NB	6.14	2.18	2.05
7	A	3017	CLA	MG-NB	6.14	2.18	2.05
7	L	3064	CLA	MG-ND	6.14	2.18	2.05
7	A	3009	CLA	MG-NB	6.14	2.18	2.05
7	B	3044	CLA	MG-NB	6.14	2.18	2.05
7	B	3011	CLA	MG-NB	6.14	2.18	2.05
7	K	3051	CLA	MG-NB	6.14	2.18	2.05
7	F	3002	CLA	MG-NB	6.14	2.18	2.05
7	A	3045	CLA	MG-NB	6.14	2.18	2.05
7	A	2502	CLA	MG-NB	6.14	2.18	2.05
7	A	3005	CLA	MG-NB	6.14	2.18	2.05
7	A	3041	CLA	MG-NB	6.13	2.18	2.05
7	B	3023	CLA	MG-NB	6.13	2.18	2.05
7	A	3027	CLA	MG-NB	6.13	2.18	2.05
7	B	3080	CLA	MG-NB	6.13	2.18	2.05
7	B	3055	CLA	MG-NB	6.12	2.18	2.05
7	B	3075	CLA	MG-NB	6.12	2.18	2.05
7	F	3012	CLA	MG-NB	6.12	2.18	2.05
7	L	3049	CLA	MG-NB	6.12	2.18	2.05
7	A	3052	CLA	MG-NB	6.12	2.18	2.05
7	B	3008	CLA	MG-NB	6.12	2.18	2.05
7	A	3024	CLA	MG-NB	6.11	2.18	2.05
7	L	3036	CLA	MG-NB	6.11	2.18	2.05
7	B	3081	CLA	MG-NB	6.11	2.18	2.05
7	A	3065	CLA	MG-NB	6.11	2.18	2.05
7	B	3076	CLA	MG-NB	6.11	2.18	2.05
7	A	3018	CLA	MG-NB	6.10	2.18	2.05
7	B	3037	CLA	MG-NB	6.10	2.18	2.05
7	B	3025	CLA	MG-NB	6.10	2.18	2.05
7	A	3013	CLA	MG-NB	6.10	2.18	2.05
7	F	3054	CLA	MG-NB	6.09	2.18	2.05
7	A	3032	CLA	MG-NB	6.09	2.18	2.05
7	A	3057	CLA	MG-NB	6.09	2.18	2.05
7	A	3062	CLA	MG-NB	6.09	2.18	2.05
7	A	3030	CLA	MG-NB	6.09	2.18	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3019	CLA	MG-NB	6.09	2.18	2.05
7	F	3033	CLA	MG-NB	6.08	2.18	2.05
7	B	2005	CLA	MG-NB	6.08	2.18	2.05
7	B	3035	CLA	MG-NB	6.07	2.18	2.05
7	F	3059	CLA	MG-NB	6.07	2.18	2.05
7	L	3038	CLA	MG-NB	6.06	2.18	2.05
7	F	3004	CLA	MG-NB	6.06	2.18	2.05
7	A	3067	CLA	MG-NB	6.06	2.18	2.05
7	B	2004	CLA	MG-NB	6.06	2.18	2.05
7	B	3042	CLA	MG-NB	6.05	2.18	2.05
7	F	3031	CLA	MG-NB	6.05	2.18	2.05
7	A	3078	CLA	MG-NB	6.04	2.18	2.05
7	K	3050	CLA	MG-NB	6.04	2.18	2.05
7	A	3079	CLA	MG-NB	6.03	2.18	2.05
7	A	2006	CLA	MG-NB	6.03	2.18	2.05
7	A	3071	CLA	MG-NB	6.03	2.18	2.05
9	C	2009	SF4	S3-FE1	-5.83	2.29	2.33
9	B	2008	SF4	S3-FE1	-5.78	2.29	2.33
7	B	2002	CLA	MG-NB	5.28	2.16	2.05
9	C	2009	SF4	S3-FE2	4.24	2.36	2.33
9	B	2008	SF4	S3-FE2	4.15	2.36	2.33
7	A	3013	CLA	C1C-NC	-3.76	1.33	1.39
7	B	2002	CLA	MG-NC	-3.76	1.96	2.07
7	L	3049	CLA	C1C-NC	-3.76	1.33	1.39
7	K	3050	CLA	C1C-NC	-3.75	1.33	1.39
7	A	3047	CLA	C1C-NC	-3.75	1.33	1.39
7	B	3003	CLA	C1C-NC	-3.75	1.33	1.39
7	B	3010	CLA	C1C-NC	-3.75	1.33	1.39
7	A	3009	CLA	C1C-NC	-3.74	1.33	1.39
7	B	2004	CLA	C1C-NC	-3.74	1.33	1.39
7	A	3065	CLA	C1C-NC	-3.74	1.33	1.39
7	A	3058	CLA	C1C-NC	-3.73	1.33	1.39
7	A	3072	CLA	C1C-NC	-3.73	1.33	1.39
7	B	2501	CLA	C1C-NC	-3.73	1.33	1.39
7	A	3071	CLA	C1C-NC	-3.73	1.33	1.39
7	F	3059	CLA	C1C-NC	-3.73	1.33	1.39
7	A	3062	CLA	C1C-NC	-3.72	1.33	1.39
7	A	3027	CLA	C1C-NC	-3.72	1.33	1.39
7	A	3077	CLA	C1C-NC	-3.72	1.33	1.39
7	A	3041	CLA	C1C-NC	-3.71	1.33	1.39
7	A	3039	CLA	C1C-NC	-3.71	1.33	1.39
7	B	3076	CLA	C1C-NC	-3.71	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3005	CLA	C1C-NC	-3.71	1.33	1.39
7	B	3075	CLA	C1C-NC	-3.71	1.33	1.39
7	L	3036	CLA	C1C-NC	-3.71	1.33	1.39
7	B	2002	CLA	C1C-NC	-3.70	1.33	1.39
7	B	3019	CLA	C1C-NC	-3.70	1.33	1.39
7	B	3037	CLA	C1C-NC	-3.70	1.33	1.39
7	A	3052	CLA	C1C-NC	-3.70	1.33	1.39
7	A	2001	CLA	MG-NC	-3.70	1.96	2.07
7	A	3007	CLA	C1C-NC	-3.70	1.33	1.39
7	A	3026	CLA	C1C-NC	-3.70	1.33	1.39
7	F	3012	CLA	C1C-NC	-3.70	1.33	1.39
7	B	3025	CLA	C1C-NC	-3.69	1.33	1.39
7	B	3001	CLA	C1C-NC	-3.69	1.33	1.39
7	F	3002	CLA	C1C-NC	-3.69	1.33	1.39
7	A	3056	CLA	C1C-NC	-3.69	1.33	1.39
7	B	2005	CLA	C1C-NC	-3.69	1.33	1.39
7	A	2006	CLA	C1C-NC	-3.68	1.33	1.39
7	A	3032	CLA	C1C-NC	-3.68	1.33	1.39
7	B	3028	CLA	C1C-NC	-3.68	1.33	1.39
7	B	3015	CLA	C1C-NC	-3.68	1.33	1.39
7	B	3063	CLA	C1C-NC	-3.68	1.33	1.39
7	B	3055	CLA	C1C-NC	-3.68	1.33	1.39
7	A	3030	CLA	C1C-NC	-3.68	1.33	1.39
7	F	3033	CLA	C1C-NC	-3.68	1.33	1.39
7	B	3046	CLA	C1C-NC	-3.67	1.33	1.39
7	A	3079	CLA	C1C-NC	-3.67	1.33	1.39
7	A	3029	CLA	C1C-NC	-3.67	1.33	1.39
7	A	3040	CLA	C1C-NC	-3.67	1.33	1.39
7	F	3004	CLA	C1C-NC	-3.67	1.33	1.39
7	K	3051	CLA	C1C-NC	-3.67	1.33	1.39
7	A	3024	CLA	C1C-NC	-3.66	1.33	1.39
7	B	3011	CLA	C1C-NC	-3.66	1.33	1.39
7	B	3023	CLA	C1C-NC	-3.66	1.33	1.39
7	A	3053	CLA	C1C-NC	-3.66	1.33	1.39
7	B	3006	CLA	C1C-NC	-3.66	1.33	1.39
7	A	3017	CLA	C1C-NC	-3.66	1.33	1.39
7	A	3018	CLA	C1C-NC	-3.66	1.33	1.39
7	A	3073	CLA	C1C-NC	-3.66	1.33	1.39
7	B	3081	CLA	C1C-NC	-3.65	1.33	1.39
7	F	3022	CLA	C1C-NC	-3.65	1.33	1.39
7	A	3021	CLA	C1C-NC	-3.65	1.33	1.39
7	B	3070	CLA	C1C-NC	-3.65	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3074	CLA	C1C-NC	-3.65	1.33	1.39
7	A	3067	CLA	C1C-NC	-3.65	1.33	1.39
7	B	3060	CLA	C1C-NC	-3.65	1.33	1.39
7	A	3045	CLA	C1C-NC	-3.65	1.33	1.39
7	A	3016	CLA	C1C-NC	-3.65	1.33	1.39
7	B	3044	CLA	C1C-NC	-3.64	1.33	1.39
7	B	3008	CLA	C1C-NC	-3.64	1.33	1.39
7	A	3078	CLA	C1C-NC	-3.64	1.33	1.39
7	A	2502	CLA	C1C-NC	-3.64	1.33	1.39
7	B	3020	CLA	C1C-NC	-3.64	1.33	1.39
7	B	3080	CLA	C1C-NC	-3.64	1.33	1.39
7	A	3048	CLA	C1C-NC	-3.63	1.33	1.39
7	A	3068	CLA	C1C-NC	-3.63	1.33	1.39
7	B	3066	CLA	C1C-NC	-3.63	1.33	1.39
7	F	3054	CLA	C1C-NC	-3.63	1.33	1.39
7	A	3043	CLA	C1C-NC	-3.63	1.33	1.39
7	B	3069	CLA	C1C-NC	-3.62	1.33	1.39
7	B	3042	CLA	C1C-NC	-3.62	1.33	1.39
7	B	3035	CLA	C1C-NC	-3.62	1.33	1.39
7	F	3031	CLA	C1C-NC	-3.62	1.33	1.39
7	L	3038	CLA	C1C-NC	-3.61	1.33	1.39
7	B	3034	CLA	C1C-NC	-3.61	1.33	1.39
7	F	3061	CLA	C1C-NC	-3.61	1.33	1.39
7	A	3057	CLA	C1C-NC	-3.58	1.33	1.39
7	B	2003	CLA	C1C-NC	-3.57	1.33	1.39
7	B	2003	CLA	MG-NC	-3.54	1.96	2.07
7	A	2001	CLA	C1C-NC	-3.52	1.34	1.39
7	B	2004	CLA	MG-NC	-3.43	1.97	2.07
7	L	3036	CLA	MG-ND	2.38	2.10	2.05
7	A	3030	CLA	MG-ND	2.38	2.10	2.05
7	K	3050	CLA	MG-ND	2.37	2.10	2.05
7	A	3057	CLA	MG-ND	2.37	2.10	2.05
7	F	3033	CLA	MG-ND	2.37	2.10	2.05
7	L	3038	CLA	MG-ND	2.36	2.10	2.05
7	A	3032	CLA	MG-ND	2.36	2.10	2.05
7	L	3049	CLA	MG-ND	2.35	2.10	2.05
7	F	3054	CLA	MG-ND	2.35	2.10	2.05
7	F	3059	CLA	MG-ND	2.35	2.10	2.05
7	A	3062	CLA	MG-ND	2.35	2.10	2.05
7	F	3012	CLA	MG-ND	2.35	2.10	2.05
7	B	3008	CLA	MG-ND	2.35	2.10	2.05
7	B	2005	CLA	MG-ND	2.35	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2006	CLA	MG-ND	2.35	2.10	2.05
7	B	3069	CLA	MG-ND	2.35	2.10	2.05
7	A	3079	CLA	MG-ND	2.35	2.10	2.05
7	A	3072	CLA	MG-ND	2.35	2.10	2.05
7	A	3071	CLA	MG-ND	2.34	2.10	2.05
7	A	3067	CLA	MG-ND	2.34	2.10	2.05
7	B	3042	CLA	MG-ND	2.34	2.10	2.05
7	A	3065	CLA	MG-ND	2.34	2.10	2.05
7	A	3078	CLA	MG-ND	2.33	2.10	2.05
7	L	3064	CLA	MG-NB	2.33	2.10	2.05
7	F	3004	CLA	MG-ND	2.33	2.10	2.05
7	B	3075	CLA	MG-ND	2.33	2.10	2.05
7	A	3007	CLA	MG-ND	2.33	2.10	2.05
7	B	3019	CLA	MG-ND	2.33	2.10	2.05
7	A	3029	CLA	MG-ND	2.32	2.10	2.05
7	B	3037	CLA	MG-ND	2.32	2.10	2.05
7	A	3013	CLA	MG-ND	2.32	2.10	2.05
7	A	3073	CLA	MG-ND	2.32	2.10	2.05
7	B	3023	CLA	MG-ND	2.32	2.10	2.05
7	A	3047	CLA	MG-ND	2.32	2.10	2.05
7	B	3080	CLA	MG-ND	2.32	2.10	2.05
7	B	3020	CLA	MG-ND	2.31	2.10	2.05
7	A	3045	CLA	MG-ND	2.31	2.10	2.05
7	B	3011	CLA	MG-ND	2.31	2.10	2.05
7	A	3024	CLA	MG-ND	2.31	2.10	2.05
7	A	3009	CLA	MG-ND	2.31	2.10	2.05
7	B	3034	CLA	MG-ND	2.31	2.10	2.05
7	B	3035	CLA	MG-ND	2.31	2.10	2.05
7	A	3014	CLA	MG-NB	2.31	2.10	2.05
7	A	3018	CLA	MG-ND	2.31	2.10	2.05
7	B	3081	CLA	MG-ND	2.31	2.10	2.05
7	B	3025	CLA	MG-ND	2.30	2.10	2.05
7	B	3074	CLA	MG-ND	2.30	2.10	2.05
7	A	3058	CLA	MG-ND	2.30	2.10	2.05
7	F	3002	CLA	MG-ND	2.30	2.10	2.05
7	F	3031	CLA	MG-ND	2.30	2.10	2.05
7	K	3051	CLA	MG-ND	2.30	2.10	2.05
7	A	3021	CLA	MG-ND	2.30	2.10	2.05
7	B	3066	CLA	MG-ND	2.30	2.10	2.05
7	A	3068	CLA	MG-ND	2.30	2.10	2.05
7	A	3017	CLA	MG-ND	2.30	2.10	2.05
7	A	3016	CLA	MG-ND	2.29	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3044	CLA	MG-ND	2.29	2.10	2.05
7	F	3022	CLA	MG-ND	2.29	2.10	2.05
7	B	3076	CLA	MG-ND	2.29	2.10	2.05
7	B	3046	CLA	MG-ND	2.29	2.10	2.05
7	B	3001	CLA	MG-ND	2.29	2.10	2.05
7	B	3003	CLA	MG-ND	2.29	2.10	2.05
7	A	3077	CLA	MG-ND	2.29	2.10	2.05
7	F	3061	CLA	MG-ND	2.29	2.10	2.05
7	A	2502	CLA	MG-ND	2.29	2.10	2.05
7	A	3040	CLA	MG-ND	2.29	2.10	2.05
7	B	3006	CLA	MG-ND	2.28	2.10	2.05
7	A	3041	CLA	MG-ND	2.28	2.10	2.05
7	A	3039	CLA	MG-ND	2.28	2.10	2.05
7	A	3043	CLA	MG-ND	2.28	2.10	2.05
7	A	3056	CLA	MG-ND	2.28	2.10	2.05
7	A	3027	CLA	MG-ND	2.28	2.10	2.05
7	B	3028	CLA	MG-ND	2.27	2.10	2.05
7	A	3052	CLA	MG-ND	2.27	2.10	2.05
7	B	3063	CLA	MG-ND	2.27	2.10	2.05
7	B	3015	CLA	MG-ND	2.27	2.10	2.05
7	B	3070	CLA	MG-ND	2.27	2.10	2.05
7	B	3055	CLA	MG-ND	2.27	2.10	2.05
7	B	3060	CLA	MG-ND	2.27	2.10	2.05
7	B	3010	CLA	MG-ND	2.27	2.10	2.05
7	A	3053	CLA	MG-ND	2.27	2.10	2.05
7	A	3026	CLA	MG-ND	2.26	2.10	2.05
7	A	3005	CLA	MG-ND	2.26	2.10	2.05
7	A	3048	CLA	MG-ND	2.25	2.10	2.05
7	B	2501	CLA	MG-ND	2.25	2.10	2.05
7	L	3064	CLA	C4C-NC	-2.13	1.33	1.37
7	A	3014	CLA	C4C-NC	-2.12	1.33	1.37

All (352) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3014	CLA	CHD-C4C-NC	12.05	133.88	124.49
7	L	3064	CLA	CHD-C4C-NC	12.03	133.87	124.49
7	A	3027	CLA	CHC-C1C-NC	5.32	133.99	123.42
7	A	3078	CLA	CHC-C1C-NC	5.32	133.98	123.42
7	A	3065	CLA	CHC-C1C-NC	5.32	133.98	123.42
7	F	3059	CLA	CHC-C1C-NC	5.32	133.98	123.42
7	A	3071	CLA	CHC-C1C-NC	5.31	133.97	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3067	CLA	CHC-C1C-NC	5.31	133.96	123.42
7	A	3062	CLA	CHC-C1C-NC	5.30	133.95	123.42
7	B	3060	CLA	CHC-C1C-NC	5.30	133.95	123.42
7	A	3021	CLA	CHC-C1C-NC	5.30	133.95	123.42
7	A	3077	CLA	CHC-C1C-NC	5.30	133.95	123.42
7	B	3006	CLA	CHC-C1C-NC	5.30	133.95	123.42
7	B	3034	CLA	CHC-C1C-NC	5.30	133.94	123.42
7	K	3050	CLA	CHC-C1C-NC	5.30	133.94	123.42
7	A	2006	CLA	CHC-C1C-NC	5.29	133.93	123.42
7	F	3002	CLA	CHC-C1C-NC	5.29	133.93	123.42
7	B	3001	CLA	CHC-C1C-NC	5.29	133.92	123.42
7	A	3009	CLA	CHC-C1C-NC	5.29	133.92	123.42
7	L	3049	CLA	CHC-C1C-NC	5.29	133.92	123.42
7	F	3004	CLA	CHC-C1C-NC	5.29	133.92	123.42
7	B	3074	CLA	CHC-C1C-NC	5.29	133.92	123.42
7	A	3045	CLA	CHC-C1C-NC	5.29	133.92	123.42
7	A	3048	CLA	CHC-C1C-NC	5.28	133.92	123.42
7	A	3072	CLA	CHC-C1C-NC	5.28	133.91	123.42
7	B	3025	CLA	CHC-C1C-NC	5.28	133.91	123.42
7	A	3024	CLA	CHC-C1C-NC	5.28	133.91	123.42
7	B	3081	CLA	CHC-C1C-NC	5.28	133.91	123.42
7	A	3043	CLA	CHC-C1C-NC	5.28	133.91	123.42
7	A	3016	CLA	CHC-C1C-NC	5.28	133.91	123.42
7	A	3017	CLA	CHC-C1C-NC	5.28	133.91	123.42
7	B	3069	CLA	CHC-C1C-NC	5.28	133.90	123.42
7	A	3079	CLA	CHC-C1C-NC	5.27	133.89	123.42
7	A	3007	CLA	CHC-C1C-NC	5.27	133.90	123.42
7	F	3022	CLA	CHC-C1C-NC	5.27	133.89	123.42
7	L	3038	CLA	CHC-C1C-NC	5.27	133.89	123.42
7	A	3026	CLA	CHC-C1C-NC	5.27	133.89	123.42
7	B	3046	CLA	CHC-C1C-NC	5.27	133.88	123.42
7	B	3008	CLA	CHC-C1C-NC	5.27	133.88	123.42
7	B	2005	CLA	CHC-C1C-NC	5.27	133.88	123.42
7	B	3023	CLA	CHC-C1C-NC	5.27	133.88	123.42
7	F	3012	CLA	CHC-C1C-NC	5.26	133.88	123.42
7	A	3073	CLA	CHC-C1C-NC	5.26	133.88	123.42
7	A	2001	CLA	CHC-C1C-NC	5.26	133.87	123.42
7	A	3032	CLA	CHC-C1C-NC	5.26	133.87	123.42
7	A	3041	CLA	CHC-C1C-NC	5.26	133.87	123.42
7	A	3056	CLA	CHC-C1C-NC	5.26	133.87	123.42
7	A	3040	CLA	CHC-C1C-NC	5.26	133.87	123.42
7	F	3033	CLA	CHC-C1C-NC	5.26	133.87	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3055	CLA	CHC-C1C-NC	5.26	133.87	123.42
7	B	3044	CLA	CHC-C1C-NC	5.26	133.87	123.42
7	A	3052	CLA	CHC-C1C-NC	5.26	133.87	123.42
7	B	3070	CLA	CHC-C1C-NC	5.26	133.86	123.42
7	A	3013	CLA	CHC-C1C-NC	5.26	133.87	123.42
7	A	3058	CLA	CHC-C1C-NC	5.26	133.86	123.42
7	B	3066	CLA	CHC-C1C-NC	5.26	133.86	123.42
7	A	3068	CLA	CHC-C1C-NC	5.25	133.85	123.42
7	A	3018	CLA	CHC-C1C-NC	5.25	133.85	123.42
7	A	2502	CLA	CHC-C1C-NC	5.25	133.85	123.42
7	B	3080	CLA	CHC-C1C-NC	5.25	133.85	123.42
7	K	3051	CLA	CHC-C1C-NC	5.25	133.85	123.42
7	F	3054	CLA	CHC-C1C-NC	5.25	133.85	123.42
7	B	3011	CLA	CHC-C1C-NC	5.25	133.85	123.42
7	B	3063	CLA	CHC-C1C-NC	5.25	133.85	123.42
7	B	3035	CLA	CHC-C1C-NC	5.25	133.84	123.42
7	B	2501	CLA	CHC-C1C-NC	5.25	133.84	123.42
7	B	3037	CLA	CHC-C1C-NC	5.25	133.84	123.42
7	B	3003	CLA	CHC-C1C-NC	5.25	133.84	123.42
7	B	3010	CLA	CHC-C1C-NC	5.25	133.84	123.42
7	B	3019	CLA	CHC-C1C-NC	5.25	133.84	123.42
7	B	3076	CLA	CHC-C1C-NC	5.24	133.84	123.42
7	B	2003	CLA	CHC-C1C-NC	5.24	133.84	123.42
7	B	3015	CLA	CHC-C1C-NC	5.24	133.84	123.42
7	F	3031	CLA	CHC-C1C-NC	5.24	133.83	123.42
7	B	3028	CLA	CHC-C1C-NC	5.24	133.83	123.42
7	A	3030	CLA	CHC-C1C-NC	5.24	133.82	123.42
7	B	3075	CLA	CHC-C1C-NC	5.23	133.82	123.42
7	A	3053	CLA	CHC-C1C-NC	5.23	133.82	123.42
7	B	2002	CLA	CHC-C1C-NC	5.23	133.81	123.42
7	B	3020	CLA	CHC-C1C-NC	5.23	133.81	123.42
7	L	3036	CLA	CHC-C1C-NC	5.23	133.81	123.42
7	F	3061	CLA	CHC-C1C-NC	5.23	133.80	123.42
7	A	3039	CLA	CHC-C1C-NC	5.22	133.79	123.42
7	A	3047	CLA	CHC-C1C-NC	5.22	133.78	123.42
7	B	3042	CLA	CHC-C1C-NC	5.22	133.78	123.42
7	A	3005	CLA	CHC-C1C-NC	5.21	133.77	123.42
7	A	3029	CLA	CHC-C1C-NC	5.21	133.77	123.42
7	B	2004	CLA	CHC-C1C-NC	5.21	133.76	123.42
7	A	3057	CLA	CHC-C1C-NC	5.20	133.75	123.42
7	F	3061	CLA	C4B-NB-C1B	4.12	111.09	107.12
7	B	3003	CLA	C4B-NB-C1B	4.12	111.09	107.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	3054	CLA	C4B-NB-C1B	4.12	111.08	107.12
7	B	3060	CLA	C4B-NB-C1B	4.10	111.06	107.12
7	B	2501	CLA	C4B-NB-C1B	4.09	111.06	107.12
7	A	3068	CLA	C4B-NB-C1B	4.09	111.06	107.12
7	B	3010	CLA	C4B-NB-C1B	4.09	111.06	107.12
7	F	3002	CLA	C4B-NB-C1B	4.09	111.06	107.12
7	B	3074	CLA	C4B-NB-C1B	4.09	111.06	107.12
7	A	3048	CLA	C4B-NB-C1B	4.09	111.05	107.12
7	B	3020	CLA	C4B-NB-C1B	4.08	111.05	107.12
7	A	3058	CLA	C4B-NB-C1B	4.08	111.05	107.12
7	A	3007	CLA	C4B-NB-C1B	4.08	111.05	107.12
7	B	3028	CLA	C4B-NB-C1B	4.08	111.05	107.12
7	F	3022	CLA	C4B-NB-C1B	4.07	111.04	107.12
7	A	3073	CLA	C4B-NB-C1B	4.07	111.04	107.12
7	B	3006	CLA	C4B-NB-C1B	4.07	111.04	107.12
7	A	3065	CLA	C4B-NB-C1B	4.06	111.03	107.12
7	A	3039	CLA	C4B-NB-C1B	4.06	111.03	107.12
7	B	3069	CLA	C4B-NB-C1B	4.06	111.03	107.12
7	A	2001	CLA	C4B-NB-C1B	4.06	111.03	107.12
7	A	3072	CLA	C4B-NB-C1B	4.06	111.03	107.12
7	A	3021	CLA	C4B-NB-C1B	4.06	111.03	107.12
7	A	3077	CLA	C4B-NB-C1B	4.06	111.02	107.12
7	A	3056	CLA	C4B-NB-C1B	4.05	111.02	107.12
7	B	3001	CLA	C4B-NB-C1B	4.05	111.02	107.12
7	B	3063	CLA	C4B-NB-C1B	4.05	111.02	107.12
7	B	3015	CLA	C4B-NB-C1B	4.04	111.01	107.12
7	A	3043	CLA	C4B-NB-C1B	4.04	111.01	107.12
7	B	3070	CLA	C4B-NB-C1B	4.04	111.00	107.12
7	A	3016	CLA	C4B-NB-C1B	4.03	111.00	107.12
7	B	3034	CLA	C4B-NB-C1B	4.03	111.00	107.12
7	A	3071	CLA	C4B-NB-C1B	4.03	111.00	107.12
7	A	3045	CLA	C4B-NB-C1B	4.03	111.00	107.12
7	A	2502	CLA	C4B-NB-C1B	4.03	111.00	107.12
7	B	2003	CLA	C4B-NB-C1B	4.03	111.00	107.12
7	A	3041	CLA	C4B-NB-C1B	4.02	110.99	107.12
7	A	3062	CLA	C4B-NB-C1B	4.02	110.99	107.12
7	F	3004	CLA	C4B-NB-C1B	4.02	110.99	107.12
7	B	3046	CLA	C4B-NB-C1B	4.02	110.99	107.12
7	B	3044	CLA	C4B-NB-C1B	4.01	110.98	107.12
7	B	3080	CLA	C4B-NB-C1B	4.01	110.98	107.12
7	F	3059	CLA	C4B-NB-C1B	4.01	110.98	107.12
7	B	3011	CLA	C4B-NB-C1B	4.01	110.98	107.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3057	CLA	C4B-NB-C1B	4.00	110.97	107.12
7	A	3029	CLA	C4B-NB-C1B	4.00	110.97	107.12
7	A	3079	CLA	C4B-NB-C1B	3.99	110.96	107.12
7	A	3053	CLA	C4B-NB-C1B	3.99	110.96	107.12
7	A	3030	CLA	C4B-NB-C1B	3.99	110.96	107.12
7	A	3047	CLA	C4B-NB-C1B	3.99	110.96	107.12
7	B	3023	CLA	C4B-NB-C1B	3.99	110.96	107.12
7	B	3037	CLA	C4B-NB-C1B	3.98	110.95	107.12
7	A	3027	CLA	C4B-NB-C1B	3.98	110.95	107.12
7	A	3017	CLA	C4B-NB-C1B	3.98	110.95	107.12
7	L	3036	CLA	C4B-NB-C1B	3.98	110.95	107.12
7	K	3051	CLA	C4B-NB-C1B	3.97	110.94	107.12
7	B	3066	CLA	C4B-NB-C1B	3.97	110.94	107.12
7	B	3081	CLA	C4B-NB-C1B	3.97	110.94	107.12
7	A	3040	CLA	C4B-NB-C1B	3.97	110.94	107.12
7	A	3026	CLA	C4B-NB-C1B	3.97	110.94	107.12
7	A	3032	CLA	C4B-NB-C1B	3.97	110.94	107.12
7	B	2005	CLA	C4B-NB-C1B	3.96	110.94	107.12
7	A	3005	CLA	C4B-NB-C1B	3.96	110.93	107.12
7	F	3012	CLA	C4B-NB-C1B	3.96	110.93	107.12
7	B	3008	CLA	C4B-NB-C1B	3.95	110.93	107.12
7	F	3033	CLA	C4B-NB-C1B	3.95	110.92	107.12
7	A	3013	CLA	C4B-NB-C1B	3.95	110.92	107.12
7	A	3052	CLA	C4B-NB-C1B	3.94	110.91	107.12
7	A	3018	CLA	C4B-NB-C1B	3.93	110.91	107.12
7	B	3035	CLA	C4B-NB-C1B	3.93	110.90	107.12
7	A	2006	CLA	C4B-NB-C1B	3.93	110.90	107.12
7	B	2004	CLA	C4B-NB-C1B	3.93	110.90	107.12
7	B	3076	CLA	C4B-NB-C1B	3.93	110.90	107.12
7	A	3024	CLA	C4B-NB-C1B	3.93	110.90	107.12
7	A	3067	CLA	C4B-NB-C1B	3.92	110.90	107.12
7	B	3025	CLA	C4B-NB-C1B	3.92	110.89	107.12
7	L	3049	CLA	C4B-NB-C1B	3.91	110.89	107.12
7	B	3019	CLA	C4B-NB-C1B	3.91	110.89	107.12
7	B	3075	CLA	C4B-NB-C1B	3.91	110.88	107.12
7	A	3009	CLA	C4B-NB-C1B	3.91	110.88	107.12
7	K	3050	CLA	C4B-NB-C1B	3.89	110.87	107.12
7	L	3038	CLA	C4B-NB-C1B	3.89	110.86	107.12
7	B	3042	CLA	C4B-NB-C1B	3.89	110.86	107.12
7	A	3078	CLA	C4B-NB-C1B	3.88	110.86	107.12
7	B	3055	CLA	C4B-NB-C1B	3.83	110.81	107.12
7	F	3031	CLA	C4B-NB-C1B	3.83	110.81	107.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2002	CLA	C4B-NB-C1B	3.78	110.76	107.12
7	L	3064	CLA	C4D-ND-C1D	3.68	111.02	106.57
7	A	3014	CLA	C4D-ND-C1D	3.69	111.02	106.57
7	L	3036	CLA	CHD-C4C-NC	-2.80	122.31	124.49
7	F	3054	CLA	CHD-C4C-NC	-2.79	122.32	124.49
7	B	2002	CLA	CHD-C4C-NC	-2.77	122.33	124.49
7	F	3033	CLA	CHD-C4C-NC	-2.75	122.35	124.49
7	B	3035	CLA	CHD-C4C-NC	-2.72	122.37	124.49
7	B	3028	CLA	CHD-C4C-NC	-2.71	122.37	124.49
7	A	3039	CLA	CHD-C4C-NC	-2.71	122.38	124.49
7	A	3032	CLA	CHD-C4C-NC	-2.71	122.38	124.49
7	B	2003	CLA	CHD-C4C-NC	-2.71	122.38	124.49
7	A	3040	CLA	CHD-C4C-NC	-2.71	122.38	124.49
7	L	3038	CLA	CHD-C4C-NC	-2.70	122.38	124.49
7	B	3042	CLA	CHD-C4C-NC	-2.70	122.38	124.49
7	A	3030	CLA	CHD-C4C-NC	-2.70	122.39	124.49
7	A	3048	CLA	CHD-C4C-NC	-2.70	122.39	124.49
7	B	3044	CLA	CHD-C4C-NC	-2.69	122.39	124.49
7	B	3015	CLA	CHD-C4C-NC	-2.68	122.40	124.49
7	B	3055	CLA	CHD-C4C-NC	-2.68	122.40	124.49
7	B	3075	CLA	CHD-C4C-NC	-2.68	122.40	124.49
7	A	3009	CLA	CHD-C4C-NC	-2.68	122.40	124.49
7	B	3081	CLA	CHD-C4C-NC	-2.68	122.40	124.49
7	A	3024	CLA	CHD-C4C-NC	-2.67	122.41	124.49
7	F	3031	CLA	CHD-C4C-NC	-2.67	122.41	124.49
7	A	2502	CLA	CHD-C4C-NC	-2.67	122.41	124.49
7	A	3027	CLA	CHD-C4C-NC	-2.67	122.41	124.49
7	A	3018	CLA	CHD-C4C-NC	-2.66	122.41	124.49
7	F	3004	CLA	CHD-C4C-NC	-2.66	122.42	124.49
7	B	3060	CLA	CHD-C4C-NC	-2.66	122.42	124.49
7	A	3005	CLA	CHD-C4C-NC	-2.65	122.42	124.49
7	A	3057	CLA	CHD-C4C-NC	-2.65	122.42	124.49
7	K	3051	CLA	CHD-C4C-NC	-2.65	122.42	124.49
7	B	3023	CLA	CHD-C4C-NC	-2.65	122.43	124.49
7	A	2006	CLA	CHD-C4C-NC	-2.64	122.43	124.49
7	B	3034	CLA	CHD-C4C-NC	-2.64	122.43	124.49
7	F	3012	CLA	CHD-C4C-NC	-2.64	122.43	124.49
7	A	3007	CLA	CHD-C4C-NC	-2.64	122.43	124.49
7	B	3025	CLA	CHD-C4C-NC	-2.64	122.43	124.49
7	A	3029	CLA	CHD-C4C-NC	-2.63	122.44	124.49
7	B	3006	CLA	CHD-C4C-NC	-2.63	122.44	124.49
7	B	3001	CLA	CHD-C4C-NC	-2.63	122.44	124.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3016	CLA	CHD-C4C-NC	-2.63	122.44	124.49
7	B	3066	CLA	CHD-C4C-NC	-2.63	122.44	124.49
7	A	3043	CLA	CHD-C4C-NC	-2.62	122.44	124.49
7	B	3010	CLA	CHD-C4C-NC	-2.62	122.45	124.49
7	A	3073	CLA	CHD-C4C-NC	-2.62	122.45	124.49
7	B	3008	CLA	CHD-C4C-NC	-2.62	122.45	124.49
7	B	2005	CLA	CHD-C4C-NC	-2.62	122.45	124.49
7	A	3026	CLA	CHD-C4C-NC	-2.62	122.45	124.49
7	B	3011	CLA	CHD-C4C-NC	-2.61	122.45	124.49
7	A	3072	CLA	CHD-C4C-NC	-2.61	122.45	124.49
7	B	3074	CLA	CHD-C4C-NC	-2.61	122.45	124.49
7	A	3021	CLA	CHD-C4C-NC	-2.61	122.46	124.49
7	L	3049	CLA	CHD-C4C-NC	-2.61	122.46	124.49
7	A	3078	CLA	CHD-C4C-NC	-2.60	122.46	124.49
7	A	3068	CLA	CHD-C4C-NC	-2.60	122.46	124.49
7	F	3002	CLA	CHD-C4C-NC	-2.60	122.46	124.49
7	F	3022	CLA	CHD-C4C-NC	-2.60	122.46	124.49
7	A	3047	CLA	CHD-C4C-NC	-2.60	122.47	124.49
7	A	3017	CLA	CHD-C4C-NC	-2.59	122.47	124.49
7	A	3013	CLA	CHD-C4C-NC	-2.59	122.47	124.49
7	A	3045	CLA	CHD-C4C-NC	-2.59	122.47	124.49
7	B	3046	CLA	CHD-C4C-NC	-2.59	122.47	124.49
7	B	3076	CLA	CHD-C4C-NC	-2.59	122.47	124.49
7	A	3052	CLA	CHD-C4C-NC	-2.59	122.47	124.49
7	A	3067	CLA	CHD-C4C-NC	-2.58	122.47	124.49
7	A	2001	CLA	CHD-C4C-NC	-2.58	122.48	124.49
7	B	3069	CLA	CHD-C4C-NC	-2.58	122.48	124.49
7	B	2501	CLA	CHD-C4C-NC	-2.58	122.48	124.49
7	A	3058	CLA	CHD-C4C-NC	-2.57	122.48	124.49
7	A	3053	CLA	CHD-C4C-NC	-2.57	122.48	124.49
7	A	3041	CLA	CHD-C4C-NC	-2.57	122.49	124.49
7	B	3019	CLA	CHD-C4C-NC	-2.57	122.49	124.49
7	A	3065	CLA	CHD-C4C-NC	-2.56	122.50	124.49
7	A	3077	CLA	CHD-C4C-NC	-2.56	122.50	124.49
7	B	3080	CLA	CHD-C4C-NC	-2.56	122.50	124.49
7	B	3003	CLA	CHD-C4C-NC	-2.55	122.50	124.49
7	A	3056	CLA	CHD-C4C-NC	-2.53	122.52	124.49
7	B	3020	CLA	CHD-C4C-NC	-2.53	122.52	124.49
7	K	3050	CLA	CHD-C4C-NC	-2.53	122.52	124.49
7	B	3037	CLA	CHD-C4C-NC	-2.53	122.52	124.49
7	B	2004	CLA	CHD-C4C-NC	-2.52	122.53	124.49
7	F	3061	CLA	CHD-C4C-NC	-2.52	122.53	124.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3062	CLA	CHD-C4C-NC	-2.51	122.53	124.49
7	A	3079	CLA	CHD-C4C-NC	-2.50	122.54	124.49
7	F	3059	CLA	CHD-C4C-NC	-2.50	122.54	124.49
7	B	3070	CLA	CHD-C4C-NC	-2.49	122.55	124.49
7	A	3071	CLA	CHD-C4C-NC	-2.49	122.55	124.49
7	B	3063	CLA	CHD-C4C-NC	-2.46	122.58	124.49
7	B	2005	CLA	C4B-CHC-C1C	-2.23	124.54	127.47
7	A	3027	CLA	C4B-CHC-C1C	-2.22	124.56	127.47
7	F	3002	CLA	C4B-CHC-C1C	-2.19	124.58	127.47
7	A	3024	CLA	C4B-CHC-C1C	-2.19	124.59	127.47
7	B	3001	CLA	C4B-CHC-C1C	-2.19	124.59	127.47
7	B	3010	CLA	C4B-CHC-C1C	-2.18	124.60	127.47
7	A	3021	CLA	C4B-CHC-C1C	-2.18	124.61	127.47
7	A	3026	CLA	C4B-CHC-C1C	-2.17	124.61	127.47
7	B	3023	CLA	C4B-CHC-C1C	-2.17	124.61	127.47
7	B	2501	CLA	C4B-CHC-C1C	-2.17	124.62	127.47
7	A	3041	CLA	C4B-CHC-C1C	-2.17	124.62	127.47
7	B	3006	CLA	C4B-CHC-C1C	-2.17	124.62	127.47
7	B	3060	CLA	C4B-CHC-C1C	-2.17	124.62	127.47
7	A	3048	CLA	C4B-CHC-C1C	-2.17	124.62	127.47
7	B	3025	CLA	C4B-CHC-C1C	-2.17	124.62	127.47
7	B	3028	CLA	C4B-CHC-C1C	-2.16	124.62	127.47
7	A	2006	CLA	C4B-CHC-C1C	-2.16	124.62	127.47
7	K	3050	CLA	C4B-CHC-C1C	-2.16	124.63	127.47
7	A	3045	CLA	C4B-CHC-C1C	-2.16	124.63	127.47
7	A	3009	CLA	C4B-CHC-C1C	-2.16	124.64	127.47
7	B	2002	CLA	C4B-CHC-C1C	-2.15	124.64	127.47
7	B	3037	CLA	C4B-CHC-C1C	-2.15	124.64	127.47
7	F	3033	CLA	C4B-CHC-C1C	-2.15	124.64	127.47
7	A	3052	CLA	C4B-CHC-C1C	-2.15	124.64	127.47
7	B	3034	CLA	C4B-CHC-C1C	-2.15	124.64	127.47
7	B	3074	CLA	C4B-CHC-C1C	-2.14	124.65	127.47
7	F	3059	CLA	C4B-CHC-C1C	-2.14	124.65	127.47
7	A	3077	CLA	C4B-CHC-C1C	-2.14	124.65	127.47
7	F	3022	CLA	C4B-CHC-C1C	-2.14	124.65	127.47
7	A	2001	CLA	C4B-CHC-C1C	-2.14	124.66	127.47
7	F	3004	CLA	C4B-CHC-C1C	-2.14	124.66	127.47
7	L	3049	CLA	C4B-CHC-C1C	-2.14	124.66	127.47
7	B	3015	CLA	C4B-CHC-C1C	-2.14	124.66	127.47
7	B	3008	CLA	C4B-CHC-C1C	-2.14	124.66	127.47
7	A	3056	CLA	C4B-CHC-C1C	-2.13	124.67	127.47
7	A	3013	CLA	C4B-CHC-C1C	-2.13	124.67	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3081	CLA	C4B-CHC-C1C	-2.13	124.67	127.47
7	B	3069	CLA	C4B-CHC-C1C	-2.13	124.67	127.47
7	B	3019	CLA	C4B-CHC-C1C	-2.13	124.67	127.47
7	B	3055	CLA	C4B-CHC-C1C	-2.13	124.67	127.47
7	A	3065	CLA	C4B-CHC-C1C	-2.13	124.67	127.47
7	B	3046	CLA	C4B-CHC-C1C	-2.13	124.67	127.47
7	A	3072	CLA	C4B-CHC-C1C	-2.12	124.68	127.47
7	L	3036	CLA	C4B-CHC-C1C	-2.12	124.68	127.47
7	A	3071	CLA	C4B-CHC-C1C	-2.12	124.68	127.47
7	A	3078	CLA	C4B-CHC-C1C	-2.12	124.69	127.47
7	B	3063	CLA	C4B-CHC-C1C	-2.12	124.68	127.47
7	B	3044	CLA	C4B-CHC-C1C	-2.11	124.69	127.47
7	A	3073	CLA	C4B-CHC-C1C	-2.11	124.69	127.47
7	A	2502	CLA	C4B-CHC-C1C	-2.11	124.69	127.47
7	F	3012	CLA	C4B-CHC-C1C	-2.11	124.69	127.47
7	A	3016	CLA	C4B-CHC-C1C	-2.11	124.69	127.47
7	A	3053	CLA	C4B-CHC-C1C	-2.11	124.69	127.47
7	A	3062	CLA	C4B-CHC-C1C	-2.11	124.69	127.47
7	K	3051	CLA	C4B-CHC-C1C	-2.11	124.69	127.47
7	B	3066	CLA	C4B-CHC-C1C	-2.11	124.69	127.47
7	A	3043	CLA	C4B-CHC-C1C	-2.11	124.70	127.47
7	L	3038	CLA	C4B-CHC-C1C	-2.11	124.70	127.47
7	A	3018	CLA	C4B-CHC-C1C	-2.11	124.70	127.47
7	B	3070	CLA	C4B-CHC-C1C	-2.11	124.70	127.47
7	A	3007	CLA	C4B-CHC-C1C	-2.11	124.70	127.47
7	A	3067	CLA	C4B-CHC-C1C	-2.11	124.70	127.47
7	B	3080	CLA	C4B-CHC-C1C	-2.10	124.70	127.47
7	A	3017	CLA	C4B-CHC-C1C	-2.10	124.70	127.47
7	A	3040	CLA	C4B-CHC-C1C	-2.10	124.71	127.47
7	A	3032	CLA	C4B-CHC-C1C	-2.10	124.70	127.47
7	B	2003	CLA	C4B-CHC-C1C	-2.10	124.71	127.47
7	A	3005	CLA	C4B-CHC-C1C	-2.10	124.71	127.47
7	B	3011	CLA	C4B-CHC-C1C	-2.10	124.71	127.47
7	F	3054	CLA	C4B-CHC-C1C	-2.10	124.71	127.47
7	F	3031	CLA	C4B-CHC-C1C	-2.10	124.71	127.47
7	B	3076	CLA	C4B-CHC-C1C	-2.10	124.71	127.47
7	B	3003	CLA	C4B-CHC-C1C	-2.10	124.71	127.47
7	F	3061	CLA	C4B-CHC-C1C	-2.10	124.71	127.47
7	B	3042	CLA	C4B-CHC-C1C	-2.09	124.72	127.47
7	A	3030	CLA	C4B-CHC-C1C	-2.09	124.72	127.47
7	A	3047	CLA	C4B-CHC-C1C	-2.09	124.73	127.47
7	A	3057	CLA	C4B-CHC-C1C	-2.09	124.72	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3035	CLA	C4B-CHC-C1C	-2.08	124.73	127.47
7	B	3020	CLA	C4B-CHC-C1C	-2.08	124.73	127.47
7	A	3029	CLA	C4B-CHC-C1C	-2.08	124.73	127.47
7	A	3068	CLA	C4B-CHC-C1C	-2.08	124.74	127.47
7	A	3058	CLA	C4B-CHC-C1C	-2.08	124.74	127.47
7	B	3075	CLA	C4B-CHC-C1C	-2.07	124.75	127.47
7	A	3039	CLA	C4B-CHC-C1C	-2.07	124.75	127.47
7	B	2004	CLA	C4B-CHC-C1C	-2.07	124.75	127.47
7	A	3079	CLA	C4B-CHC-C1C	-2.06	124.77	127.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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