



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 06:49 AM GMT

PDB ID : 1QZV
Title : Crystal structure of plant photosystem I
Authors : Ben-Shem, A.; Frolow, F.; Nelson, N.
Deposited on : 2003-09-18
Resolution : 4.44 Å(reported)

This is a wwPDB validation summary 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>

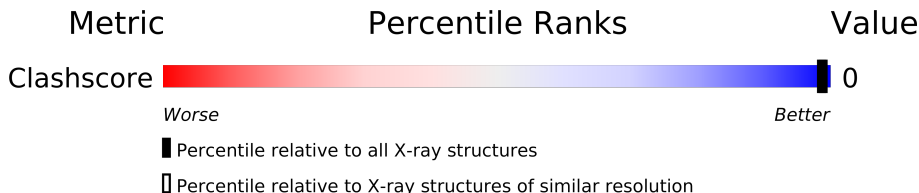
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.44 Å.








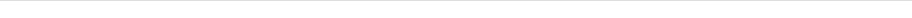




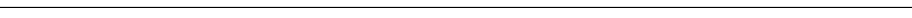







Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1285 (5.30-3.50)










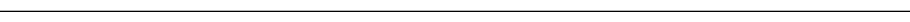

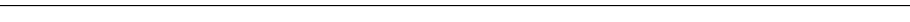
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The 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	726	
1	P	726	
2	B	732	
2	Q	732	
3	C	80	
3	R	80	
4	D	154	
4	S	154	
5	E	64	
5	T	64	
6	F	154	
6	U	154	
7	G	74	
7	V	74	
8	H	52	
8	W	52	
9	I	30	
9	Y	30	
10	J	41	
10	Z	41	

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Mol	Chain	Length	Quality of chain
11	5	42	
11	K	42	
12	6	135	
12	L	135	
13	1	109	
13	7	109	
14	2	115	
14	8	115	
15	3	117	
15	9	117	
16	0	119	
16	4	119	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 13938 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 PLANT PHOTOSYSTEM I: SUBUNIT PSAA.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	726	Total	C	0	0	726
			726	726			
1	P	726	Total	C	0	0	726
			726	726			

- Molecule 2 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAB.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	732	Total	C	0	0	732
			732	732			
2	Q	732	Total	C	0	0	732
			732	732			

- Molecule 3 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAC.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	80	Total	C	0	0	80
			80	80			
3	R	80	Total	C	0	0	80
			80	80			

- Molecule 4 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAD.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	D	154	Total	C	0	0	154
			154	154			
4	S	154	Total	C	0	0	154
			154	154			

- Molecule 5 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	64	Total C 64 64	0	0	64
5	T	64	Total C 64 64	0	0	64

- Molecule 6 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAF.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	154	Total C 154 154	0	0	154
6	U	154	Total C 154 154	0	0	154

- Molecule 7 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAG.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	74	Total C 74 74	0	0	74
7	V	74	Total C 74 74	0	0	74

- Molecule 8 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAH.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	52	Total C 52 52	0	0	52
8	W	52	Total C 52 52	0	0	52

- Molecule 9 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAL.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	30	Total C 30 30	0	0	30
9	Y	30	Total C 30 30	0	0	30

- Molecule 10 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAJ.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	41	Total C 41 41	0	0	41

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	Z	41	Total C 41 41	0	0	41

- Molecule 11 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAK.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	K	42	Total C 42 42	0	0	42
11	5	42	Total C 42 42	0	0	42

- Molecule 12 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAL.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	L	135	Total C 135 135	0	0	135
12	6	135	Total C 135 135	0	0	135

- Molecule 13 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	1	109	Total C 109 109	0	0	109
13	7	109	Total C 109 109	0	0	109

- Molecule 14 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	2	115	Total C 115 115	0	0	115
14	8	115	Total C 115 115	0	0	115

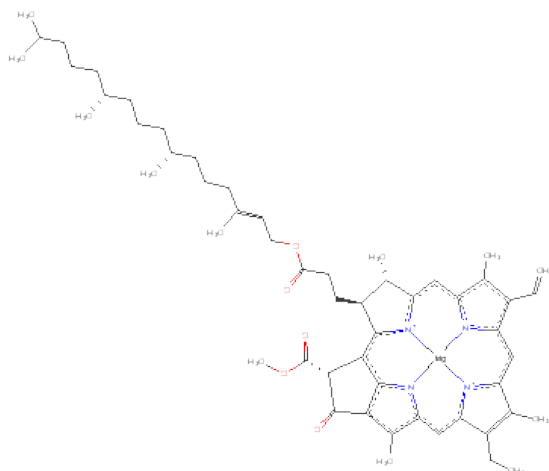
- Molecule 15 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	3	117	Total C 117 117	0	0	117
15	9	117	Total C 117 117	0	0	117

- Molecule 16 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	4	119	Total C 119 119	0	0	119
16	0	119	Total C 119 119	0	0	119

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	J	1	Total 25	C 20	Mg 1	N 4	0	0
17	K	1	Total 25	C 20	Mg 1	N 4	0	0
17	A	1	Total 25	C 20	Mg 1	N 4	0	0
17	K	1	Total 25	C 20	Mg 1	N 4	0	0
17	K	1	Total 25	C 20	Mg 1	N 4	0	0
17	L	1	Total 25	C 20	Mg 1	N 4	0	0
17	L	1	Total 25	C 20	Mg 1	N 4	0	0
17	L	1	Total 25	C 20	Mg 1	N 4	0	0
17	L	1	Total 25	C 20	Mg 1	N 4	0	0
17	G	1	Total 25	C 20	Mg 1	N 4	0	0
17	H	1	Total 25	C 20	Mg 1	N 4	0	0
17	A	1	Total 25	C 20	Mg 1	N 4	0	0
17	B	1	Total 25	C 20	Mg 1	N 4	0	0
17	4	1	Total 25	C 20	Mg 1	N 4	0	0
17	F	1	Total 25	C 20	Mg 1	N 4	0	0
17	F	1	Total 25	C 20	Mg 1	N 4	0	0
17	F	1	Total 25	C 20	Mg 1	N 4	0	0
17	F	1	Total 25	C 20	Mg 1	N 4	0	0
17	2	1	Total 25	C 20	Mg 1	N 4	0	0
17	J	1	Total 25	C 20	Mg 1	N 4	0	0
17	A	1	Total 25	C 20	Mg 1	N 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	U	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	V	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	Q	1	Total 25	C 20	Mg 1	N 4	0	0
17	U	1	Total 25	C 20	Mg 1	N 4	0	0
17	Z	1	Total 25	C 20	Mg 1	N 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	V	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	W	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Z	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		

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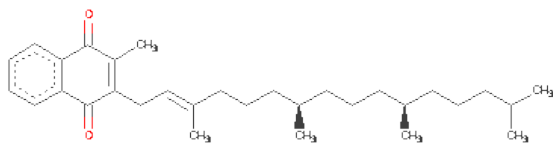
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		

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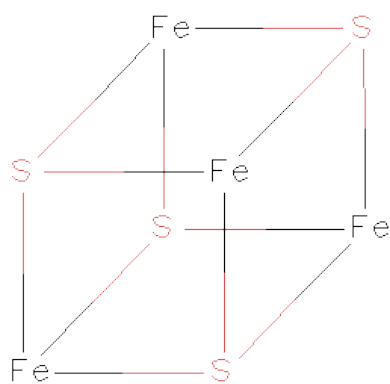
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			13	11	2		
18	B	1	Total	C	O	0	0
			13	11	2		
18	P	1	Total	C	O	0	0
			13	11	2		
18	Q	1	Total	C	O	0	0
			13	11	2		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total 8	Fe 4	S 4	0	0
19	C	1	Total 8	Fe 4	S 4	0	0
19	C	1	Total 8	Fe 4	S 4	0	0
19	P	1	Total 8	Fe 4	S 4	0	0
19	R	1	Total 8	Fe 4	S 4	0	0
19	R	1	Total 8	Fe 4	S 4	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain A: 

There are no outlier residues recorded for this chain.

- Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain P: 

There are no outlier residues recorded for this chain.

- Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain B: 



- Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain Q: 



- Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain C: 

There are no outlier residues recorded for this chain.

- Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain R: 

There are no outlier residues recorded for this chain.

- Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain D: 

There are no outlier residues recorded for this chain.

- Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain S: 

There are no outlier residues recorded for this chain.

- Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain E: 

There are no outlier residues recorded for this chain.

- Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain T: 

There are no outlier residues recorded for this chain.

- Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain F: 

There are no outlier residues recorded for this chain.

- Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain U: 

There are no outlier residues recorded for this chain.

- Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain G: 

There are no outlier residues recorded for this chain.

- Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain V: 

There are no outlier residues recorded for this chain.

- Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain H: 

There are no outlier residues recorded for this chain.

- Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain W: 

There are no outlier residues recorded for this chain.

- Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain I: 

There are no outlier residues recorded for this chain.

- Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain Y: 

There are no outlier residues recorded for this chain.

- Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain J: 

There are no outlier residues recorded for this chain.

- Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain Z: 

There are no outlier residues recorded for this chain.

- Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain K: 

There are no outlier residues recorded for this chain.

- Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain 5: 

There are no outlier residues recorded for this chain.

- Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain L: 

There are no outlier residues recorded for this chain.

- Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain 6: 

There are no outlier residues recorded for this chain.

- Molecule 13: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1

Chain 1: 

There are no outlier residues recorded for this chain.

- Molecule 13: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1

Chain 7: 

There are no outlier residues recorded for this chain.

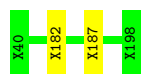
- Molecule 14: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2

Chain 2: 



- Molecule 14: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2

Chain 8: 



- Molecule 15: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA3

Chain 3: 

There are no outlier residues recorded for this chain.

- Molecule 15: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA3

Chain 9: 

There are no outlier residues recorded for this chain.

- Molecule 16: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA4

Chain 4: 

There are no outlier residues recorded for this chain.

- Molecule 16: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA4

Chain 0: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	182.28Å 190.38Å 220.25Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	50.00 – 4.44	Depositor
% Data completeness (in resolution range)	99.6 (50.00-4.44)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.410 , 0.420	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13938	wwPDB-VP
Average B, all atoms (Å ²)	105.0	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5

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	726	0	0	0	0
1	P	726	0	0	0	0
2	B	732	0	0	1	0
2	Q	732	0	0	1	0
3	C	80	0	0	0	0
3	R	80	0	0	0	0
4	D	154	0	0	0	0
4	S	154	0	0	0	0
5	E	64	0	0	0	0
5	T	64	0	0	0	0
6	F	154	0	0	0	0
6	U	154	0	0	0	0
7	G	74	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	V	74	0	0	0	0
8	H	52	0	0	0	0
8	W	52	0	0	0	0
9	I	30	0	0	0	0
9	Y	30	0	0	0	0
10	J	41	0	0	0	0
10	Z	41	0	0	0	0
11	5	42	0	0	0	0
11	K	42	0	0	0	0
12	6	135	0	0	0	0
12	L	135	0	0	0	0
13	1	109	0	0	0	0
13	7	109	0	0	0	0
14	2	115	0	0	1	0
14	8	115	0	0	1	0
15	3	117	0	0	0	0
15	9	117	0	0	0	0
16	0	119	0	0	0	0
16	4	119	0	0	0	0
17	0	400	0	48	0	0
17	1	325	0	39	0	0
17	2	375	0	45	0	0
17	3	350	0	42	0	0
17	4	400	0	48	0	0
17	5	75	0	9	0	0
17	6	100	0	12	0	0
17	7	325	0	39	0	0
17	8	375	0	45	0	0
17	9	350	0	42	0	0
17	A	1125	0	135	0	0
17	B	1125	0	135	0	0
17	F	150	0	18	0	0
17	G	50	0	6	0	0
17	H	25	0	3	0	0
17	J	75	0	9	0	0
17	K	75	0	9	0	0
17	L	100	0	12	0	0
17	P	1125	0	135	0	0
17	Q	1125	0	135	0	0
17	U	150	0	18	0	0
17	V	50	0	6	0	0
17	W	25	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Z	75	0	9	0	0
18	A	13	0	7	0	0
18	B	13	0	7	0	0
18	P	13	0	7	0	0
18	Q	13	0	7	0	0
19	A	8	0	0	0	0
19	C	16	0	0	0	0
19	P	8	0	0	0	0
19	R	16	0	0	0	0
All	All	13938	0	1030	4	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 0.

All (4) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:8:182:UNK:CA	14:8:187:UNK:CA	2.92	0.48
14:2:182:UNK:CA	14:2:187:UNK:CA	2.92	0.47
2:B:5:UNK:CA	2:B:6:UNK:CA	2.97	0.42
2:Q:5:UNK:CA	2:Q:6:UNK:CA	2.97	0.42

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

344 ligands are modelled in this entry.

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$
17	CLA	0	1011	-	23,32,73	21.00	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	0	1012	-	23,32,73	21.06	11 (47%)	12,54,113	1.82	3 (25%)
17	CLA	0	1013	-	23,32,73	20.97	10 (43%)	12,54,113	1.79	2 (16%)
17	CLA	0	1014	-	23,32,73	20.90	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	0	1015	-	23,32,73	21.13	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	0	1016	-	23,32,73	21.10	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	0	1017	-	23,32,73	20.91	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	0	1021	-	23,32,73	21.03	11 (47%)	12,54,113	1.77	2 (16%)
17	CLA	0	1022	-	23,32,73	21.22	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	0	1023	-	23,32,73	20.77	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	0	1025	-	23,32,73	20.87	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	0	1026	-	23,32,73	21.02	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	0	1031	-	23,32,73	21.00	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	0	1032	-	23,32,73	21.02	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	0	1033	-	23,32,73	20.97	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	0	8002	-	23,32,73	21.03	12 (52%)	12,54,113	1.83	2 (16%)
17	CLA	1	1011	-	23,32,73	21.00	12 (52%)	12,54,113	1.82	2 (16%)
17	CLA	1	1012	-	23,32,73	20.92	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	1	1013	-	23,32,73	20.96	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	1	1014	-	23,32,73	20.95	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1015	-	23,32,73	20.87	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1016	-	23,32,73	20.94	11 (47%)	12,54,113	1.79	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	1	1017	-	23,32,73	21.01	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1021	-	23,32,73	21.00	12 (52%)	12,54,113	1.79	2 (16%)
17	CLA	1	1022	-	23,32,73	20.84	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1023	-	23,32,73	21.11	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	1	1025	-	23,32,73	20.95	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1026	-	23,32,73	20.72	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	1	1031	-	23,32,73	20.85	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	2	1011	-	23,32,73	20.99	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	2	1012	-	23,32,73	20.87	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	2	1013	-	23,32,73	20.93	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	2	1014	-	23,32,73	20.81	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	2	1015	-	23,32,73	20.87	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	2	1016	-	23,32,73	20.86	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	2	1017	-	23,32,73	21.21	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	2	1021	-	23,32,73	20.83	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	2	1022	-	23,32,73	21.09	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	2	1023	-	23,32,73	20.94	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	2	1025	-	23,32,73	20.98	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	2	1026	-	23,32,73	20.91	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	2	1031	-	23,32,73	20.95	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	2	1033	-	23,32,73	21.01	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	2	4007	-	23,32,73	20.97	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1011	-	23,32,73	21.00	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	3	1012	-	23,32,73	20.91	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	3	1014	-	23,32,73	20.92	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	3	1015	-	23,32,73	20.95	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1016	-	23,32,73	20.94	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	3	1017	-	23,32,73	20.95	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1021	-	23,32,73	21.00	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1022	-	23,32,73	20.89	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	3	1025	-	23,32,73	20.77	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1026	-	23,32,73	20.94	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1031	-	23,32,73	20.91	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	3	1032	-	23,32,73	21.08	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	3	1033	-	23,32,73	20.91	11 (47%)	12,54,113	1.82	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	3	1041	-	23,32,73	20.97	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1011	-	23,32,73	21.10	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	4	1012	-	23,32,73	21.17	11 (47%)	12,54,113	1.83	3 (25%)
17	CLA	4	1013	-	23,32,73	21.01	10 (43%)	12,54,113	1.80	2 (16%)
17	CLA	4	1014	-	23,32,73	20.88	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	4	1015	-	23,32,73	21.14	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1016	-	23,32,73	21.00	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1017	-	23,32,73	20.82	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	4	1021	-	23,32,73	20.99	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	4	1022	-	23,32,73	21.09	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1023	-	23,32,73	20.86	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	4	1025	-	23,32,73	20.89	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	4	1026	-	23,32,73	21.06	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1031	-	23,32,73	21.04	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	4	1032	-	23,32,73	21.00	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	1033	-	23,32,73	21.07	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	4	4002	-	23,32,73	21.00	12 (52%)	12,54,113	1.82	2 (16%)
17	CLA	5	5401	-	23,32,73	20.98	11 (47%)	12,54,113	1.63	2 (16%)
17	CLA	5	5403	-	23,32,73	21.06	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	5	5404	-	23,32,73	21.11	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	6	5501	-	23,32,73	22.22	10 (43%)	12,54,113	1.60	2 (16%)
17	CLA	6	5502	-	23,32,73	20.90	10 (43%)	12,54,113	1.74	2 (16%)
17	CLA	6	5503	-	23,32,73	19.82	9 (39%)	12,54,113	1.62	2 (16%)
17	CLA	6	5504	-	23,32,73	20.92	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	7	1011	-	23,32,73	21.00	12 (52%)	12,54,113	1.82	2 (16%)
17	CLA	7	1012	-	23,32,73	20.97	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	7	1013	-	23,32,73	20.95	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	7	1014	-	23,32,73	20.89	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	7	1015	-	23,32,73	20.83	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	7	1016	-	23,32,73	20.89	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	7	1017	-	23,32,73	21.05	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	7	1021	-	23,32,73	20.97	12 (52%)	12,54,113	1.79	2 (16%)
17	CLA	7	1022	-	23,32,73	20.88	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	7	1023	-	23,32,73	20.98	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	7	1025	-	23,32,73	20.97	11 (47%)	12,54,113	1.81	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	7	1026	-	23,32,73	20.71	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	7	1031	-	23,32,73	20.93	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	8	1011	-	23,32,73	21.04	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	8	1012	-	23,32,73	20.84	12 (52%)	12,54,113	1.82	2 (16%)
17	CLA	8	1013	-	23,32,73	20.91	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	8	1014	-	23,32,73	20.83	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	8	1015	-	23,32,73	20.90	12 (52%)	12,54,113	1.80	2 (16%)
17	CLA	8	1016	-	23,32,73	20.93	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	8	1017	-	23,32,73	21.13	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	8	1021	-	23,32,73	20.88	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	8	1022	-	23,32,73	21.09	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	8	1023	-	23,32,73	20.95	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	8	1025	-	23,32,73	21.07	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	8	1026	-	23,32,73	20.92	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	8	1031	-	23,32,73	20.90	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	8	1033	-	23,32,73	21.08	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	8	8007	-	23,32,73	20.93	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	9	1011	-	23,32,73	21.06	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	9	1012	-	23,32,73	20.79	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	9	1014	-	23,32,73	20.91	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	9	1015	-	23,32,73	20.90	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	9	1016	-	23,32,73	20.93	11 (47%)	12,54,113	1.78	2 (16%)
17	CLA	9	1017	-	23,32,73	20.91	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	9	1021	-	23,32,73	20.96	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	9	1022	-	23,32,73	20.86	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	9	1025	-	23,32,73	20.73	10 (43%)	12,54,113	1.80	2 (16%)
17	CLA	9	1026	-	23,32,73	21.02	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	9	1031	-	23,32,73	20.96	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	9	1032	-	23,32,73	21.08	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	9	1033	-	23,32,73	21.05	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	9	1041	-	23,32,73	20.97	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	A	1011	-	23,32,73	20.99	9 (39%)	12,54,113	1.62	1 (8%)
17	CLA	A	1012	-	23,32,73	19.06	10 (43%)	12,54,113	1.78	3 (25%)
17	CLA	A	1013	-	23,32,73	20.55	12 (52%)	12,54,113	1.54	2 (16%)
17	CLA	A	1102	-	23,32,73	18.40	10 (43%)	12,54,113	1.68	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	1103	-	23,32,73	19.31	11 (47%)	12,54,113	1.92	2 (16%)
17	CLA	A	1104	-	23,32,73	20.57	10 (43%)	12,54,113	1.72	2 (16%)
17	CLA	A	1105	-	23,32,73	20.20	10 (43%)	12,54,113	1.56	1 (8%)
17	CLA	A	1106	-	23,32,73	20.10	11 (47%)	12,54,113	1.77	3 (25%)
17	CLA	A	1107	-	23,32,73	18.31	10 (43%)	12,54,113	1.72	1 (8%)
17	CLA	A	1108	-	23,32,73	18.46	11 (47%)	12,54,113	2.42	6 (50%)
17	CLA	A	1109	-	23,32,73	20.16	11 (47%)	12,54,113	1.64	2 (16%)
17	CLA	A	1110	-	23,32,73	21.30	10 (43%)	12,54,113	1.83	2 (16%)
17	CLA	A	1111	-	23,32,73	21.45	11 (47%)	12,54,113	1.86	3 (25%)
17	CLA	A	1112	-	23,32,73	22.18	12 (52%)	12,54,113	1.65	2 (16%)
17	CLA	A	1113	-	23,32,73	19.93	12 (52%)	12,54,113	2.63	5 (41%)
17	CLA	A	1114	-	23,32,73	19.70	11 (47%)	12,54,113	1.69	2 (16%)
17	CLA	A	1115	-	23,32,73	21.67	10 (43%)	12,54,113	1.51	1 (8%)
17	CLA	A	1116	-	23,32,73	19.94	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	A	1117	-	23,32,73	17.11	9 (39%)	12,54,113	1.62	2 (16%)
17	CLA	A	1118	-	23,32,73	22.19	10 (43%)	12,54,113	1.89	3 (25%)
17	CLA	A	1119	-	23,32,73	18.96	11 (47%)	12,54,113	1.72	2 (16%)
17	CLA	A	1120	-	23,32,73	20.55	10 (43%)	12,54,113	1.74	2 (16%)
17	CLA	A	1121	-	23,32,73	20.36	12 (52%)	12,54,113	1.51	2 (16%)
17	CLA	A	1122	-	23,32,73	18.64	12 (52%)	12,54,113	1.70	2 (16%)
17	CLA	A	1123	-	23,32,73	21.12	10 (43%)	12,54,113	1.79	2 (16%)
17	CLA	A	1124	-	23,32,73	18.53	10 (43%)	12,54,113	1.62	2 (16%)
17	CLA	A	1125	-	23,32,73	22.07	10 (43%)	12,54,113	1.87	3 (25%)
17	CLA	A	1126	-	23,32,73	20.20	10 (43%)	12,54,113	1.63	2 (16%)
17	CLA	A	1127	-	23,32,73	17.68	11 (47%)	12,54,113	1.62	1 (8%)
17	CLA	A	1128	-	23,32,73	22.26	10 (43%)	12,54,113	1.60	2 (16%)
17	CLA	A	1129	-	23,32,73	20.30	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	A	1131	-	23,32,73	17.18	11 (47%)	12,54,113	1.68	2 (16%)
17	CLA	A	1132	-	23,32,73	16.86	10 (43%)	12,54,113	1.68	2 (16%)
17	CLA	A	1133	-	23,32,73	18.64	10 (43%)	12,54,113	1.74	2 (16%)
17	CLA	A	1134	-	23,32,73	21.35	10 (43%)	12,54,113	1.78	2 (16%)
17	CLA	A	1135	-	23,32,73	21.15	9 (39%)	12,54,113	1.77	2 (16%)
17	CLA	A	1136	-	23,32,73	23.08	11 (47%)	12,54,113	1.59	2 (16%)
17	CLA	A	1137	-	23,32,73	20.60	12 (52%)	12,54,113	2.43	5 (41%)
17	CLA	A	1138	-	23,32,73	21.46	10 (43%)	12,54,113	1.79	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	1139	-	23,32,73	18.64	9 (39%)	12,54,113	1.59	1 (8%)
17	CLA	A	1140	-	23,32,73	20.86	10 (43%)	12,54,113	1.78	2 (16%)
17	CLA	A	1402	-	23,32,73	21.14	9 (39%)	12,54,113	1.80	2 (16%)
17	CLA	A	1901	-	23,32,73	20.66	12 (52%)	12,54,113	2.77	5 (41%)
18	PQN	A	2001	-	12,14,34	6.26	8 (66%)	15,20,45	0.70	0
19	SF4	A	3001	-	12,12,12	7.84	12 (100%)	0,24,24	0.00	-
17	CLA	A	4009	-	23,32,73	20.89	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	A	4010	-	23,32,73	21.00	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	B	1021	-	23,32,73	19.22	10 (43%)	12,54,113	1.66	2 (16%)
17	CLA	B	1022	-	23,32,73	19.72	11 (47%)	12,54,113	1.80	3 (25%)
17	CLA	B	1023	-	23,32,73	23.86	13 (56%)	12,54,113	1.73	2 (16%)
17	CLA	B	1130	-	23,32,73	21.55	10 (43%)	12,54,113	1.78	2 (16%)
17	CLA	B	1201	-	23,32,73	19.93	9 (39%)	12,54,113	1.75	3 (25%)
17	CLA	B	1202	-	23,32,73	18.97	8 (34%)	12,54,113	1.78	2 (16%)
17	CLA	B	1203	-	23,32,73	20.90	9 (39%)	12,54,113	1.71	2 (16%)
17	CLA	B	1204	-	23,32,73	21.17	11 (47%)	12,54,113	1.85	2 (16%)
17	CLA	B	1205	-	23,32,73	21.40	11 (47%)	12,54,113	1.55	1 (8%)
17	CLA	B	1206	-	23,32,73	15.62	8 (34%)	12,54,113	1.77	1 (8%)
17	CLA	B	1207	-	23,32,73	21.70	9 (39%)	12,54,113	1.72	2 (16%)
17	CLA	B	1208	-	23,32,73	20.35	11 (47%)	12,54,113	1.66	2 (16%)
17	CLA	B	1209	-	23,32,73	21.78	11 (47%)	12,54,113	1.71	2 (16%)
17	CLA	B	1210	-	23,32,73	21.00	12 (52%)	12,54,113	1.79	2 (16%)
17	CLA	B	1211	-	23,32,73	18.88	11 (47%)	12,54,113	1.65	2 (16%)
17	CLA	B	1212	-	23,32,73	21.03	11 (47%)	12,54,113	1.63	1 (8%)
17	CLA	B	1213	-	23,32,73	21.22	11 (47%)	12,54,113	1.60	2 (16%)
17	CLA	B	1214	-	23,32,73	20.35	11 (47%)	12,54,113	1.70	2 (16%)
17	CLA	B	1215	-	23,32,73	18.07	9 (39%)	12,54,113	1.72	2 (16%)
17	CLA	B	1216	-	23,32,73	19.35	12 (52%)	12,54,113	1.59	2 (16%)
17	CLA	B	1217	-	23,32,73	20.45	10 (43%)	12,54,113	1.76	2 (16%)
17	CLA	B	1218	-	23,32,73	21.63	10 (43%)	12,54,113	1.77	2 (16%)
17	CLA	B	1219	-	23,32,73	22.30	12 (52%)	12,54,113	2.52	4 (33%)
17	CLA	B	1220	-	23,32,73	21.13	9 (39%)	12,54,113	1.69	2 (16%)
17	CLA	B	1221	-	23,32,73	21.65	11 (47%)	12,54,113	1.90	3 (25%)
17	CLA	B	1222	-	23,32,73	19.22	9 (39%)	12,54,113	1.68	2 (16%)
17	CLA	B	1223	-	23,32,73	20.97	11 (47%)	12,54,113	1.82	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	1224	-	23,32,73	20.87	10 (43%)	12,54,113	1.74	2 (16%)
17	CLA	B	1225	-	23,32,73	18.23	10 (43%)	12,54,113	1.40	1 (8%)
17	CLA	B	1226	-	23,32,73	18.91	11 (47%)	12,54,113	1.58	2 (16%)
17	CLA	B	1227	-	23,32,73	19.68	12 (52%)	12,54,113	1.74	2 (16%)
17	CLA	B	1228	-	23,32,73	21.38	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	B	1230	-	23,32,73	20.32	11 (47%)	12,54,113	1.66	2 (16%)
17	CLA	B	1231	-	23,32,73	22.48	11 (47%)	12,54,113	1.83	2 (16%)
17	CLA	B	1232	-	23,32,73	21.88	11 (47%)	12,54,113	1.68	2 (16%)
17	CLA	B	1234	-	23,32,73	21.07	9 (39%)	12,54,113	1.72	2 (16%)
17	CLA	B	1235	-	23,32,73	21.26	11 (47%)	12,54,113	1.70	2 (16%)
17	CLA	B	1236	-	23,32,73	18.39	11 (47%)	12,54,113	1.60	2 (16%)
17	CLA	B	1237	-	23,32,73	18.51	9 (39%)	12,54,113	1.74	2 (16%)
17	CLA	B	1238	-	23,32,73	18.13	9 (39%)	12,54,113	1.58	1 (8%)
17	CLA	B	1239	-	23,32,73	17.34	9 (39%)	12,54,113	1.71	2 (16%)
17	CLA	B	1240	-	23,32,73	20.90	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	B	1241	-	23,32,73	20.95	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	B	1242	-	23,32,73	21.02	11 (47%)	12,54,113	1.79	2 (16%)
18	PQN	B	2002	-	12,14,34	6.05	8 (66%)	15,20,45	0.80	0
17	CLA	B	4001	-	23,32,73	20.94	11 (47%)	12,54,113	1.81	2 (16%)
19	SF4	C	3002	-	12,12,12	10.20	10 (83%)	0,24,24	0.00	-
19	SF4	C	3003	-	12,12,12	5.85	11 (91%)	0,24,24	0.00	-
17	CLA	F	1229	-	23,32,73	20.37	10 (43%)	12,54,113	1.72	2 (16%)
17	CLA	F	1301	-	23,32,73	21.93	11 (47%)	12,54,113	1.62	1 (8%)
17	CLA	F	4003	-	23,32,73	20.72	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	F	4004	-	23,32,73	20.97	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	F	4005	-	23,32,73	20.93	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	F	4006	-	23,32,73	20.97	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	G	1233	-	23,32,73	21.03	10 (43%)	12,54,113	1.72	2 (16%)
17	CLA	G	1701	-	23,32,73	20.98	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	H	1801	-	23,32,73	21.03	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	J	1101	-	23,32,73	20.96	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	J	1302	-	23,32,73	20.11	12 (52%)	12,54,113	2.70	6 (50%)
17	CLA	J	4008	-	23,32,73	20.98	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	K	1401	-	23,32,73	21.04	11 (47%)	12,54,113	1.64	2 (16%)
17	CLA	K	1403	-	23,32,73	21.03	11 (47%)	12,54,113	1.80	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	K	1404	-	23,32,73	21.10	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	L	1501	-	23,32,73	22.13	10 (43%)	12,54,113	1.59	2 (16%)
17	CLA	L	1502	-	23,32,73	20.90	10 (43%)	12,54,113	1.72	2 (16%)
17	CLA	L	1503	-	23,32,73	19.73	10 (43%)	12,54,113	1.62	2 (16%)
17	CLA	L	1504	-	23,32,73	20.89	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	P	5011	-	23,32,73	21.12	9 (39%)	12,54,113	1.62	1 (8%)
17	CLA	P	5012	-	23,32,73	19.10	10 (43%)	12,54,113	1.77	3 (25%)
17	CLA	P	5013	-	23,32,73	20.63	12 (52%)	12,54,113	1.54	2 (16%)
17	CLA	P	5102	-	23,32,73	18.40	10 (43%)	12,54,113	1.67	2 (16%)
17	CLA	P	5103	-	23,32,73	19.30	11 (47%)	12,54,113	1.92	2 (16%)
17	CLA	P	5104	-	23,32,73	20.59	10 (43%)	12,54,113	1.72	2 (16%)
17	CLA	P	5105	-	23,32,73	20.22	10 (43%)	12,54,113	1.56	1 (8%)
17	CLA	P	5106	-	23,32,73	20.09	11 (47%)	12,54,113	1.77	3 (25%)
17	CLA	P	5107	-	23,32,73	18.53	10 (43%)	12,54,113	1.71	1 (8%)
17	CLA	P	5108	-	23,32,73	18.52	10 (43%)	12,54,113	2.42	6 (50%)
17	CLA	P	5109	-	23,32,73	20.13	11 (47%)	12,54,113	1.65	2 (16%)
17	CLA	P	5110	-	23,32,73	21.23	10 (43%)	12,54,113	1.84	3 (25%)
17	CLA	P	5111	-	23,32,73	21.54	11 (47%)	12,54,113	1.86	3 (25%)
17	CLA	P	5112	-	23,32,73	22.22	12 (52%)	12,54,113	1.64	2 (16%)
17	CLA	P	5113	-	23,32,73	20.06	12 (52%)	12,54,113	2.63	5 (41%)
17	CLA	P	5114	-	23,32,73	19.72	11 (47%)	12,54,113	1.69	2 (16%)
17	CLA	P	5115	-	23,32,73	21.68	10 (43%)	12,54,113	1.51	1 (8%)
17	CLA	P	5116	-	23,32,73	19.87	10 (43%)	12,54,113	1.79	2 (16%)
17	CLA	P	5117	-	23,32,73	17.11	9 (39%)	12,54,113	1.62	1 (8%)
17	CLA	P	5118	-	23,32,73	22.14	10 (43%)	12,54,113	1.89	3 (25%)
17	CLA	P	5119	-	23,32,73	18.97	12 (52%)	12,54,113	1.72	2 (16%)
17	CLA	P	5120	-	23,32,73	20.54	10 (43%)	12,54,113	1.74	2 (16%)
17	CLA	P	5121	-	23,32,73	20.36	12 (52%)	12,54,113	1.52	2 (16%)
17	CLA	P	5122	-	23,32,73	18.73	12 (52%)	12,54,113	1.71	2 (16%)
17	CLA	P	5123	-	23,32,73	21.08	10 (43%)	12,54,113	1.80	2 (16%)
17	CLA	P	5124	-	23,32,73	18.46	10 (43%)	12,54,113	1.64	2 (16%)
17	CLA	P	5125	-	23,32,73	22.14	10 (43%)	12,54,113	1.87	3 (25%)
17	CLA	P	5126	-	23,32,73	20.23	11 (47%)	12,54,113	1.63	2 (16%)
17	CLA	P	5127	-	23,32,73	17.71	10 (43%)	12,54,113	1.62	1 (8%)
17	CLA	P	5128	-	23,32,73	22.35	10 (43%)	12,54,113	1.61	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	P	5129	-	23,32,73	20.39	10 (43%)	12,54,113	1.81	2 (16%)
17	CLA	P	5131	-	23,32,73	17.24	11 (47%)	12,54,113	1.67	2 (16%)
17	CLA	P	5132	-	23,32,73	16.79	10 (43%)	12,54,113	1.67	2 (16%)
17	CLA	P	5133	-	23,32,73	18.67	10 (43%)	12,54,113	1.73	2 (16%)
17	CLA	P	5134	-	23,32,73	21.36	10 (43%)	12,54,113	1.78	2 (16%)
17	CLA	P	5135	-	23,32,73	21.20	9 (39%)	12,54,113	1.75	2 (16%)
17	CLA	P	5136	-	23,32,73	23.15	11 (47%)	12,54,113	1.59	2 (16%)
17	CLA	P	5137	-	23,32,73	20.73	12 (52%)	12,54,113	2.44	5 (41%)
17	CLA	P	5138	-	23,32,73	21.45	10 (43%)	12,54,113	1.80	3 (25%)
17	CLA	P	5139	-	23,32,73	18.59	9 (39%)	12,54,113	1.59	1 (8%)
17	CLA	P	5140	-	23,32,73	20.82	10 (43%)	12,54,113	1.78	2 (16%)
17	CLA	P	5402	-	23,32,73	21.22	9 (39%)	12,54,113	1.80	2 (16%)
17	CLA	P	5901	-	23,32,73	20.70	12 (52%)	12,54,113	2.76	5 (41%)
18	PQN	P	6001	-	12,14,34	6.26	9 (75%)	15,20,45	0.70	0
19	SF4	P	7001	-	12,12,12	7.86	12 (100%)	0,24,24	0.00	-
17	CLA	P	8009	-	23,32,73	20.83	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	P	8010	-	23,32,73	20.98	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	Q	5021	-	23,32,73	19.29	10 (43%)	12,54,113	1.65	2 (16%)
17	CLA	Q	5022	-	23,32,73	19.71	11 (47%)	12,54,113	1.79	3 (25%)
17	CLA	Q	5023	-	23,32,73	23.84	13 (56%)	12,54,113	1.74	2 (16%)
17	CLA	Q	5130	-	23,32,73	21.61	10 (43%)	12,54,113	1.79	2 (16%)
17	CLA	Q	5201	-	23,32,73	19.84	9 (39%)	12,54,113	1.75	3 (25%)
17	CLA	Q	5202	-	23,32,73	19.06	8 (34%)	12,54,113	1.78	2 (16%)
17	CLA	Q	5203	-	23,32,73	21.09	9 (39%)	12,54,113	1.73	2 (16%)
17	CLA	Q	5204	-	23,32,73	21.13	11 (47%)	12,54,113	1.85	2 (16%)
17	CLA	Q	5205	-	23,32,73	21.34	11 (47%)	12,54,113	1.56	1 (8%)
17	CLA	Q	5206	-	23,32,73	15.64	8 (34%)	12,54,113	1.77	1 (8%)
17	CLA	Q	5207	-	23,32,73	21.69	9 (39%)	12,54,113	1.73	2 (16%)
17	CLA	Q	5208	-	23,32,73	20.25	11 (47%)	12,54,113	1.65	2 (16%)
17	CLA	Q	5209	-	23,32,73	21.71	11 (47%)	12,54,113	1.70	2 (16%)
17	CLA	Q	5210	-	23,32,73	20.97	12 (52%)	12,54,113	1.78	2 (16%)
17	CLA	Q	5211	-	23,32,73	18.81	11 (47%)	12,54,113	1.66	2 (16%)
17	CLA	Q	5212	-	23,32,73	21.06	11 (47%)	12,54,113	1.64	1 (8%)
17	CLA	Q	5213	-	23,32,73	21.29	11 (47%)	12,54,113	1.60	2 (16%)
17	CLA	Q	5214	-	23,32,73	20.45	10 (43%)	12,54,113	1.71	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	Q	5215	-	23,32,73	17.98	9 (39%)	12,54,113	1.73	2 (16%)
17	CLA	Q	5216	-	23,32,73	19.35	12 (52%)	12,54,113	1.59	2 (16%)
17	CLA	Q	5217	-	23,32,73	20.50	10 (43%)	12,54,113	1.76	2 (16%)
17	CLA	Q	5218	-	23,32,73	21.61	10 (43%)	12,54,113	1.76	2 (16%)
17	CLA	Q	5219	-	23,32,73	22.25	12 (52%)	12,54,113	2.52	4 (33%)
17	CLA	Q	5220	-	23,32,73	21.18	9 (39%)	12,54,113	1.70	2 (16%)
17	CLA	Q	5221	-	23,32,73	21.57	11 (47%)	12,54,113	1.90	3 (25%)
17	CLA	Q	5222	-	23,32,73	19.26	10 (43%)	12,54,113	1.68	2 (16%)
17	CLA	Q	5223	-	23,32,73	20.98	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	Q	5224	-	23,32,73	20.91	10 (43%)	12,54,113	1.73	2 (16%)
17	CLA	Q	5225	-	23,32,73	18.29	10 (43%)	12,54,113	1.41	1 (8%)
17	CLA	Q	5226	-	23,32,73	18.93	10 (43%)	12,54,113	1.57	2 (16%)
17	CLA	Q	5227	-	23,32,73	19.77	12 (52%)	12,54,113	1.74	2 (16%)
17	CLA	Q	5228	-	23,32,73	21.50	11 (47%)	12,54,113	1.83	2 (16%)
17	CLA	Q	5230	-	23,32,73	20.30	11 (47%)	12,54,113	1.66	2 (16%)
17	CLA	Q	5231	-	23,32,73	22.37	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	Q	5232	-	23,32,73	21.76	11 (47%)	12,54,113	1.67	2 (16%)
17	CLA	Q	5234	-	23,32,73	21.04	9 (39%)	12,54,113	1.71	2 (16%)
17	CLA	Q	5235	-	23,32,73	21.21	11 (47%)	12,54,113	1.70	2 (16%)
17	CLA	Q	5236	-	23,32,73	18.30	11 (47%)	12,54,113	1.61	2 (16%)
17	CLA	Q	5237	-	23,32,73	18.49	9 (39%)	12,54,113	1.75	2 (16%)
17	CLA	Q	5238	-	23,32,73	18.09	9 (39%)	12,54,113	1.59	2 (16%)
17	CLA	Q	5239	-	23,32,73	17.32	9 (39%)	12,54,113	1.71	2 (16%)
17	CLA	Q	5240	-	23,32,73	20.84	11 (47%)	12,54,113	1.79	2 (16%)
17	CLA	Q	5241	-	23,32,73	20.90	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	Q	5242	-	23,32,73	21.04	11 (47%)	12,54,113	1.79	2 (16%)
18	PQN	Q	6002	-	12,14,34	6.06	7 (58%)	15,20,45	0.80	0
17	CLA	Q	8001	-	23,32,73	20.89	11 (47%)	12,54,113	1.81	2 (16%)
19	SF4	R	7002	-	12,12,12	10.16	10 (83%)	0,24,24	0.00	-
19	SF4	R	7003	-	12,12,12	5.84	11 (91%)	0,24,24	0.00	-
17	CLA	U	5229	-	23,32,73	20.40	10 (43%)	12,54,113	1.73	2 (16%)
17	CLA	U	5301	-	23,32,73	21.82	11 (47%)	12,54,113	1.62	1 (8%)
17	CLA	U	8003	-	23,32,73	20.62	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	U	8004	-	23,32,73	20.96	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	U	8005	-	23,32,73	21.02	11 (47%)	12,54,113	1.81	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	U	8006	-	23,32,73	20.87	11 (47%)	12,54,113	1.81	2 (16%)
17	CLA	V	5233	-	23,32,73	21.06	10 (43%)	12,54,113	1.71	2 (16%)
17	CLA	V	5701	-	23,32,73	21.01	11 (47%)	12,54,113	1.82	2 (16%)
17	CLA	W	5801	-	23,32,73	21.06	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	Z	5101	-	23,32,73	20.95	11 (47%)	12,54,113	1.80	2 (16%)
17	CLA	Z	5302	-	23,32,73	20.10	12 (52%)	12,54,113	2.70	5 (41%)
17	CLA	Z	8008	-	23,32,73	21.07	11 (47%)	12,54,113	1.81	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
17	CLA	0	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1032	-	-	0/0/66/135	0/0/8/9
17	CLA	0	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	0	8002	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1025	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	1	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	2	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	2	4007	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1032	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	3	1041	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1025	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	4	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1032	-	-	0/0/66/135	0/0/8/9
17	CLA	4	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	4	4002	-	-	0/0/66/135	0/0/8/9
17	CLA	5	5401	-	-	0/0/66/135	0/0/8/9
17	CLA	5	5403	-	-	0/0/66/135	0/0/8/9
17	CLA	5	5404	-	-	0/0/66/135	0/0/8/9
17	CLA	6	5501	-	-	0/0/66/135	0/0/8/9
17	CLA	6	5502	-	-	0/0/66/135	0/0/8/9
17	CLA	6	5503	-	-	0/0/66/135	0/0/8/9
17	CLA	6	5504	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	7	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	8	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	8	8007	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1012	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	9	1014	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1015	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1016	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1017	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1025	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1026	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1031	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1032	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1033	-	-	0/0/66/135	0/0/8/9
17	CLA	9	1041	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1011	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1012	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1013	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1102	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1103	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1104	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1105	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1106	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1107	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1108	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1109	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1110	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1111	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1112	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1113	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1114	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1115	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1116	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1117	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1118	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1119	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1120	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1121	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1122	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1123	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1124	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1125	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1126	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1127	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1128	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	1129	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1131	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1132	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1133	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1134	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1135	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1136	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1137	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1138	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1139	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1140	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1402	-	-	0/0/66/135	0/0/8/9
17	CLA	A	1901	-	-	0/0/66/135	0/0/8/9
18	PQN	A	2001	-	-	0/0/16/43	0/0/2/2
19	SF4	A	3001	-	-	0/0/48/48	0/0/5/5
17	CLA	A	4009	-	-	0/0/66/135	0/0/8/9
17	CLA	A	4010	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1021	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1022	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1023	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1130	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1201	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1202	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1203	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1204	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1205	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1206	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1207	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1208	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1209	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1210	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1211	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1212	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1213	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1214	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1215	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1216	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1217	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1218	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1219	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1220	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1221	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	1222	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1223	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1224	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1225	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1226	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1227	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1228	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1230	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1231	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1232	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1234	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1235	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1236	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1237	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1238	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1239	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1240	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1241	-	-	0/0/66/135	0/0/8/9
17	CLA	B	1242	-	-	0/0/66/135	0/0/8/9
18	PQN	B	2002	-	-	0/0/16/43	0/0/2/2
17	CLA	B	4001	-	-	0/0/66/135	0/0/8/9
19	SF4	C	3002	-	-	0/0/48/48	0/0/5/5
19	SF4	C	3003	-	-	0/0/48/48	0/0/5/5
17	CLA	F	1229	-	-	0/0/66/135	0/0/8/9
17	CLA	F	1301	-	-	0/0/66/135	0/0/8/9
17	CLA	F	4003	-	-	0/0/66/135	0/0/8/9
17	CLA	F	4004	-	-	0/0/66/135	0/0/8/9
17	CLA	F	4005	-	-	0/0/66/135	0/0/8/9
17	CLA	F	4006	-	-	0/0/66/135	0/0/8/9
17	CLA	G	1233	-	-	0/0/66/135	0/0/8/9
17	CLA	G	1701	-	-	0/0/66/135	0/0/8/9
17	CLA	H	1801	-	-	0/0/66/135	0/0/8/9
17	CLA	J	1101	-	-	0/0/66/135	0/0/8/9
17	CLA	J	1302	-	-	0/0/66/135	0/0/8/9
17	CLA	J	4008	-	-	0/0/66/135	0/0/8/9
17	CLA	K	1401	-	-	0/0/66/135	0/0/8/9
17	CLA	K	1403	-	-	0/0/66/135	0/0/8/9
17	CLA	K	1404	-	-	0/0/66/135	0/0/8/9
17	CLA	L	1501	-	-	0/0/66/135	0/0/8/9
17	CLA	L	1502	-	-	0/0/66/135	0/0/8/9
17	CLA	L	1503	-	-	0/0/66/135	0/0/8/9
17	CLA	L	1504	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	P	5011	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5012	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5013	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5102	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5103	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5104	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5105	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5106	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5107	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5108	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5109	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5110	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5111	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5112	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5113	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5114	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5115	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5116	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5117	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5118	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5119	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5120	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5121	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5122	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5123	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5124	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5125	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5126	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5127	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5128	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5129	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5131	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5132	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5133	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5134	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5135	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5136	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5137	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5138	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5139	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5140	-	-	0/0/66/135	0/0/8/9
17	CLA	P	5402	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	P	5901	-	-	0/0/66/135	0/0/8/9
18	PQN	P	6001	-	-	0/0/16/43	0/0/2/2
19	SF4	P	7001	-	-	0/0/48/48	0/0/5/5
17	CLA	P	8009	-	-	0/0/66/135	0/0/8/9
17	CLA	P	8010	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5021	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5022	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5023	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5130	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5201	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5202	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5203	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5204	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5205	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5206	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5207	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5208	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5209	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5210	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5211	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5212	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5213	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5214	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5215	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5216	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5217	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5218	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5219	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5220	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5221	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5222	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5223	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5224	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5225	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5226	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5227	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5228	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5230	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5231	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5232	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5234	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5235	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	Q	5236	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5237	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5238	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5239	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5240	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5241	-	-	0/0/66/135	0/0/8/9
17	CLA	Q	5242	-	-	0/0/66/135	0/0/8/9
18	PQN	Q	6002	-	-	0/0/16/43	0/0/2/2
17	CLA	Q	8001	-	-	0/0/66/135	0/0/8/9
19	SF4	R	7002	-	-	0/0/48/48	0/0/5/5
19	SF4	R	7003	-	-	0/0/48/48	0/0/5/5
17	CLA	U	5229	-	-	0/0/66/135	0/0/8/9
17	CLA	U	5301	-	-	0/0/66/135	0/0/8/9
17	CLA	U	8003	-	-	0/0/66/135	0/0/8/9
17	CLA	U	8004	-	-	0/0/66/135	0/0/8/9
17	CLA	U	8005	-	-	0/0/66/135	0/0/8/9
17	CLA	U	8006	-	-	0/0/66/135	0/0/8/9
17	CLA	V	5233	-	-	0/0/66/135	0/0/8/9
17	CLA	V	5701	-	-	0/0/66/135	0/0/8/9
17	CLA	W	5801	-	-	0/0/66/135	0/0/8/9
17	CLA	Z	5101	-	-	0/0/66/135	0/0/8/9
17	CLA	Z	5302	-	-	0/0/66/135	0/0/8/9
17	CLA	Z	8008	-	-	0/0/66/135	0/0/8/9

The worst 5 of 3669 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1023	CLA	C3B-C4B	87.74	1.50	1.38
17	Q	5023	CLA	C3B-C4B	87.40	1.50	1.38
17	B	1232	CLA	C3B-C4B	82.18	1.49	1.38
17	Q	5232	CLA	C3B-C4B	81.88	1.49	1.38
17	P	5128	CLA	C3B-C4B	81.50	1.49	1.38

The worst 5 of 702 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Z	5302	CLA	C4A-NA-C1A	6.10	114.24	106.22
17	J	1302	CLA	C4A-NA-C1A	6.09	114.22	106.22
17	A	1901	CLA	C4A-NA-C1A	5.96	114.05	106.22
17	P	5901	CLA	C4A-NA-C1A	5.95	114.03	106.22
17	A	1113	CLA	C4A-NA-C1A	5.67	113.67	106.22

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.