



# wwPDB X-ray Structure Validation Summary 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 wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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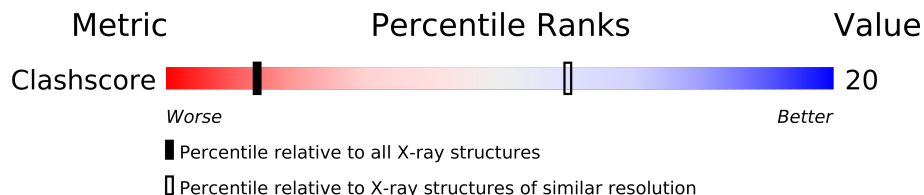
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 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  $\geq 3$ , 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			

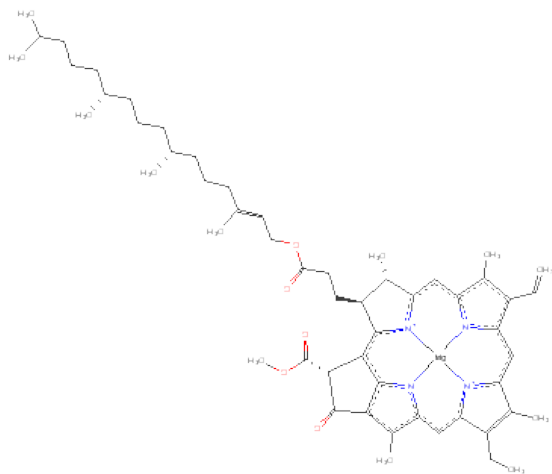
- Molecule 5 is a protein called PHOTOSYSTEM I.

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



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 25	C 20	Mg 1	N 4	0	0
7	L	1	Total 25	C 20	Mg 1	N 4	0	0
7	K	1	Total 25	C 20	Mg 1	N 4	0	0
7	K	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	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	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	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	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	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

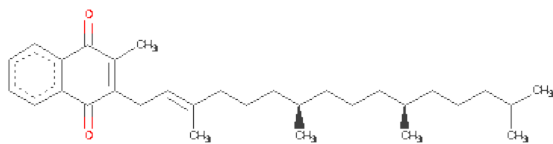
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C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

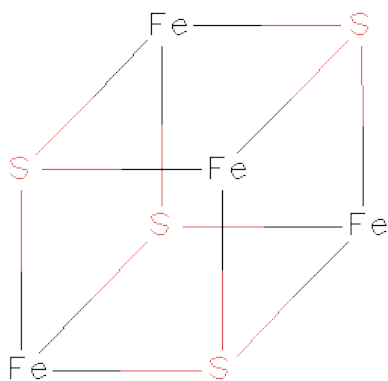
- Molecule 8 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).





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<sub>4</sub>S<sub>4</sub>).



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: 



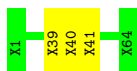
- Molecule 3: PHOTOSYSTEM I

Chain L: 

There are no outlier residues recorded for this chain.

- Molecule 4: PHOTOSYSTEM I

Chain K: 



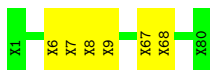
- Molecule 5: PHOTOSYSTEM I

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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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.

The worst 5 of 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

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%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

The worst 5 of 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

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.