



wwPDB X-ray Structure Validation Summary Report

Jun 17, 2014 – 06:03 PM EDT

PDB ID : 4L6V
Title : Crystal structure of a virus like photosystem I from the cyanobacterium Synechocystis PCC 6803
Authors : Mazor, Y.; Nataf, D.; Toporik, H.; Nelson, N.
Deposited on : 2013-06-13
Resolution : 3.80 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>

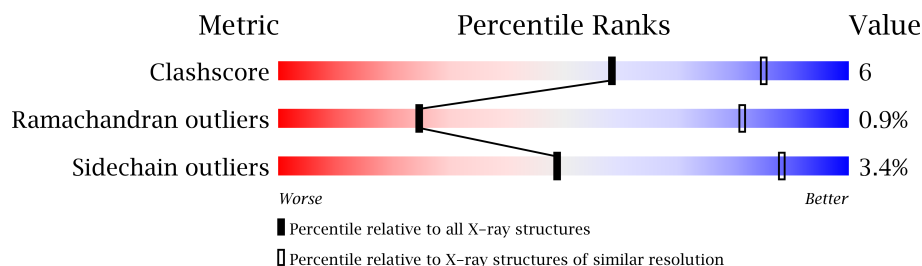
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23161

1 Overall quality at a glance

The reported resolution of this entry is 3.80 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	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)






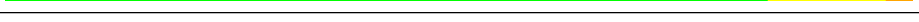

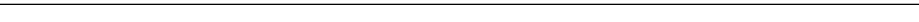




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	751	
1	A	751	
1	a	751	
2	2	731	
2	B	731	
2	b	731	
3	3	81	
3	C	81	
3	c	81	
4	4	141	
4	D	141	
4	d	141	
5	5	74	
5	E	74	
5	e	74	
6	6	125	

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Mol	Chain	Length	Quality of chain
6	F	125	
6	f	125	
7	8	157	
7	L	157	
7	l	157	
8	7	31	
8	M	31	
8	m	31	
9	9	40	
9	I	40	
9	i	40	
10	0	128	
10	K	128	
10	k	128	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 68370 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	a	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	1	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			
2	b	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			
2	2	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			
3	c	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			
3	3	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			

- Molecule 4 is a protein called Photosystem I subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			
4	4	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	68	Total	C	N	O		0	0	0
			529	332	93	104				
5	e	68	Total	C	N	O		0	0	0
			529	332	93	104				
5	5	68	Total	C	N	O		0	0	0
			529	332	93	104				

- Molecule 6 is a protein called Fusion protein of Photosystem I subunit III and subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	125	Total	C	N	O		0	0	0
			676	420	126	130				
6	f	125	Total	C	N	O		0	0	0
			685	429	126	130				
6	6	125	Total	C	N	O		0	0	0
			685	429	126	130				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	41	CYS	-	LINKER	UNP L8AII8
F	42	SER	-	LINKER	UNP L8AII8
F	43	CYS	-	LINKER	UNP L8AII8
F	53	ILE	LEU	engineered mutation	UNP L8AII8
f	41	CYS	-	LINKER	UNP L8AII8
f	42	SER	-	LINKER	UNP L8AII8
f	43	CYS	-	LINKER	UNP L8AII8
f	53	ILE	LEU	engineered mutation	UNP L8AII8
6	41	CYS	-	LINKER	UNP L8AII8
6	42	SER	-	LINKER	UNP L8AII8
6	43	CYS	-	LINKER	UNP L8AII8
6	53	ILE	LEU	engineered mutation	UNP L8AII8

- Molecule 7 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			
7	l	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			
7	8	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			

- Molecule 8 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	31	Total	C	N	O	0	0	0
			235	157	36	42			
8	m	31	Total	C	N	O	0	0	0
			235	157	36	42			
8	7	31	Total	C	N	O	0	0	0
			235	157	36	42			

- Molecule 9 is a protein called Photosystem I subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	i	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			
9	9	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			
9	I	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			

- Molecule 10 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			
10	k	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			
10	0	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	L	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	a	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	a	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	a	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	a	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	a	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	a	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	a	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
11	a	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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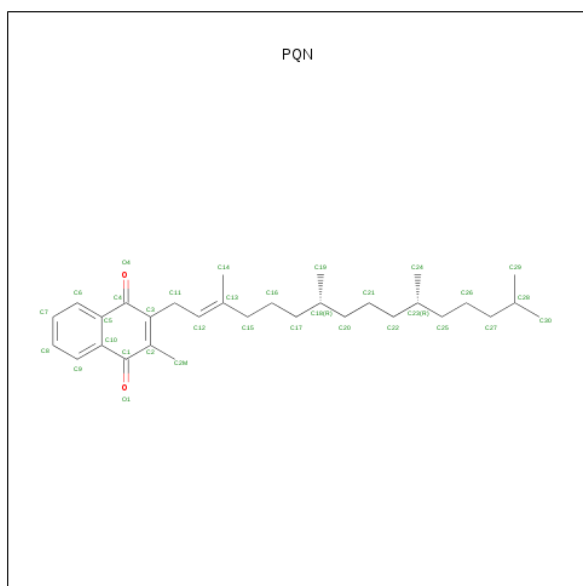
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	8	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	8	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	k	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	k	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	0	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 12 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



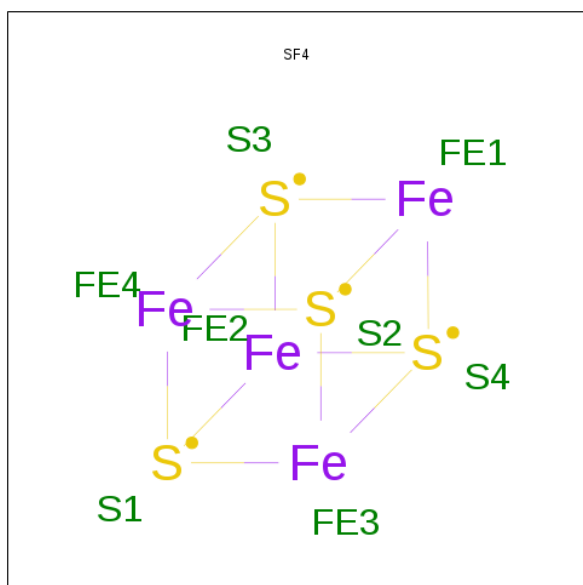
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			33	31	2		
12	B	1	Total	C	O	0	0
			33	31	2		
12	a	1	Total	C	O	0	0
			33	31	2		
12	b	1	Total	C	O	0	0
			33	31	2		

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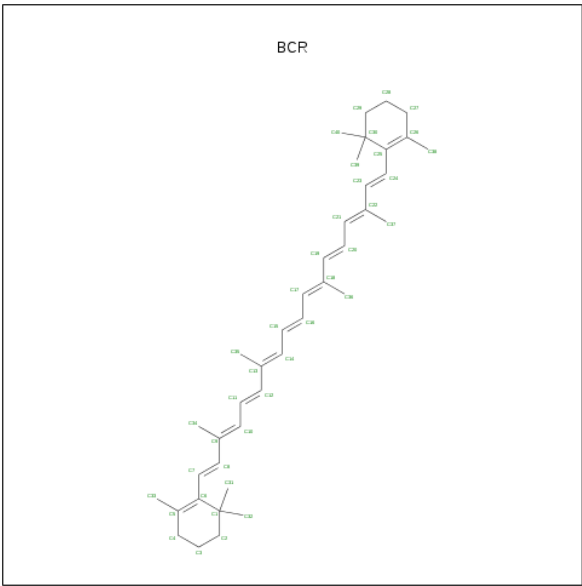
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	1	1	Total	C	O	0	0
			33	31	2		
12	2	1	Total	C	O	0	0
			33	31	2		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	Fe	S	0	0
			8	4	4		
13	C	1	Total	Fe	S	0	0
			8	4	4		
13	C	1	Total	Fe	S	0	0
			8	4	4		
13	a	1	Total	Fe	S	0	0
			8	4	4		
13	c	1	Total	Fe	S	0	0
			8	4	4		
13	c	1	Total	Fe	S	0	0
			8	4	4		
13	1	1	Total	Fe	S	0	0
			8	4	4		
13	3	1	Total	Fe	S	0	0
			8	4	4		
13	3	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	L	1	Total C 40 40	0	0
14	L	1	Total C 40 40	0	0
14	M	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	f	1	Total C 40 40	0	0
14	f	1	Total C 40 40	0	0

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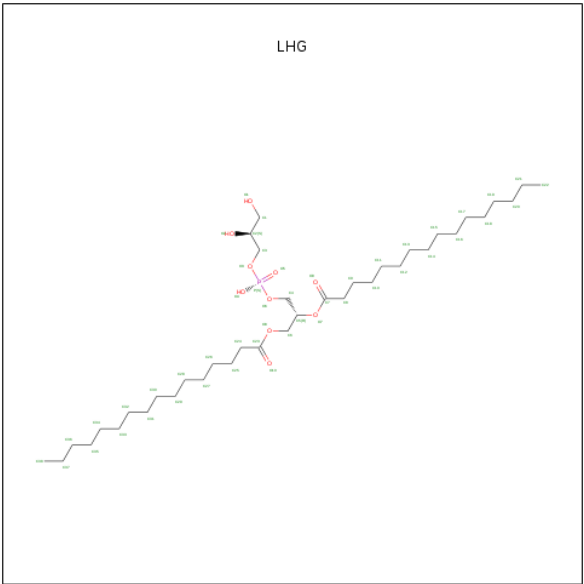
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	f	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	m	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	8	1	Total C 40 40	0	0

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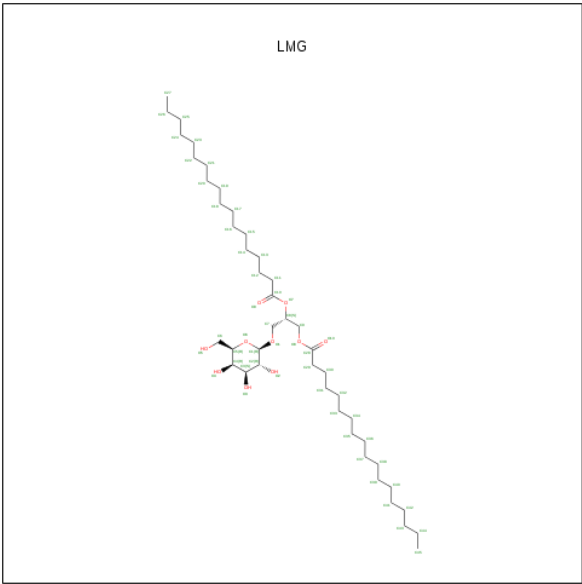
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	8	1	Total C 40 40	0	0
14	7	1	Total C 40 40	0	0

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C O P 49 38 10 1	0	0
15	A	1	Total C O P 49 38 10 1	0	0
15	B	1	Total C O P 49 38 10 1	0	0
15	a	1	Total C O P 49 38 10 1	0	0
15	a	1	Total C O P 49 38 10 1	0	0
15	b	1	Total C O P 49 38 10 1	0	0
15	1	1	Total C O P 49 38 10 1	0	0
15	1	1	Total C O P 49 38 10 1	0	0
15	2	1	Total C O P 49 38 10 1	0	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



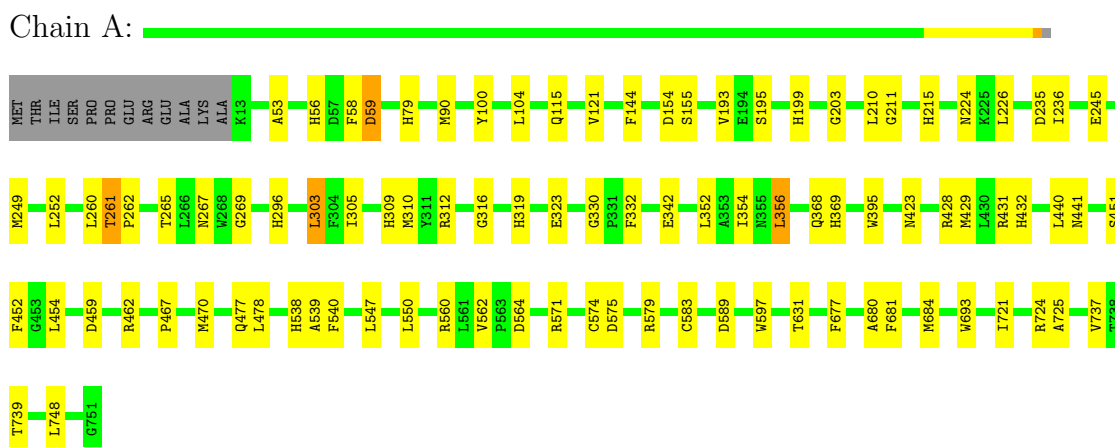
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	C	O	0	0
			55	45	10		
16	b	1	Total	C	O	0	0
			55	45	10		
16	2	1	Total	C	O	0	0
			55	45	10		

3 Residue-property plots

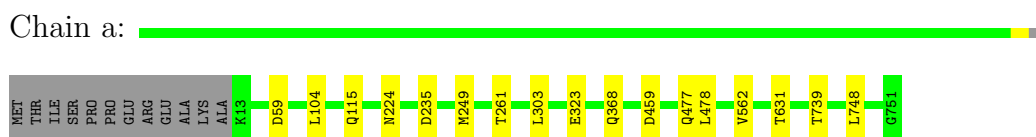
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 failed to run properly.

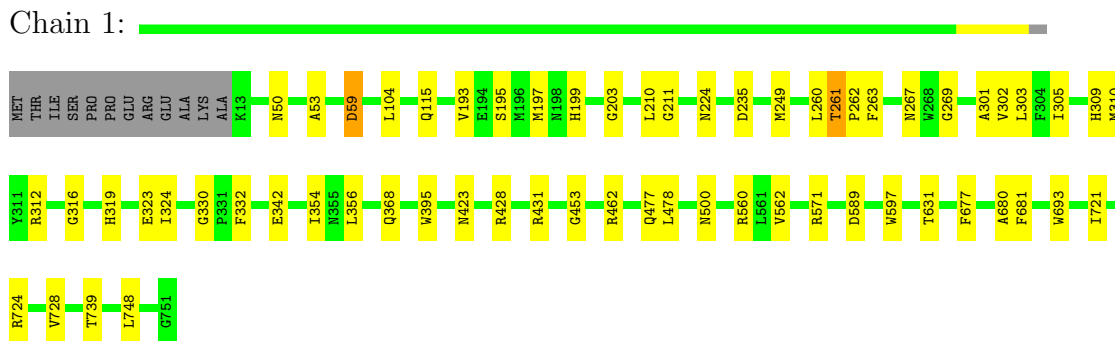
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





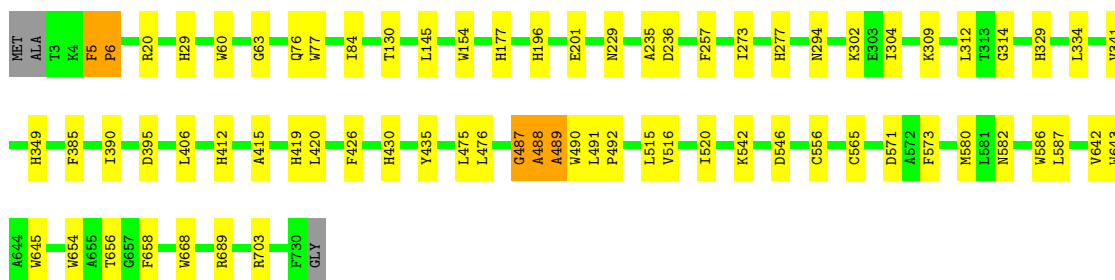
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



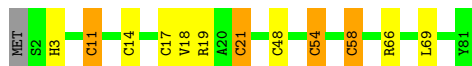
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2:



- Molecule 3: Photosystem I iron-sulfur center

Chain C:



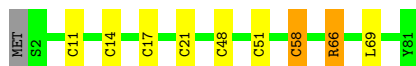
- Molecule 3: Photosystem I iron-sulfur center

Chain c:



- Molecule 3: Photosystem I iron-sulfur center

Chain 3:



- Molecule 4: Photosystem I subunit II

Chain D:



- Molecule 4: Photosystem I subunit II

Chain d:



- Molecule 4: Photosystem I subunit II

Chain 4:



- Molecule 5: Photosystem I reaction center subunit IV

Chain E:



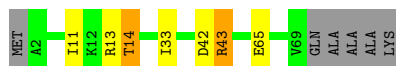
- Molecule 5: Photosystem I reaction center subunit IV

Chain e:



- Molecule 5: Photosystem I reaction center subunit IV

Chain 5:



- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain F:



- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain f:



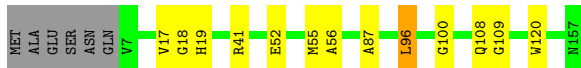
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX

Chain 6:



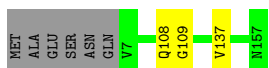
- Molecule 7: Photosystem I reaction center subunit XI

Chain L:



- Molecule 7: Photosystem I reaction center subunit XI

Chain l:



- Molecule 7: Photosystem I reaction center subunit XI

Chain 8:



- Molecule 8: Photosystem I reaction center subunit XII

Chain M:



- Molecule 8: Photosystem I reaction center subunit XII

Chain m:



- Molecule 8: Photosystem I reaction center subunit XII

Chain 7:



- Molecule 9: Photosystem I subunit III

Chain i:



- Molecule 9: Photosystem I subunit III

Chain 9:



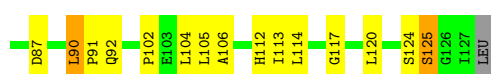
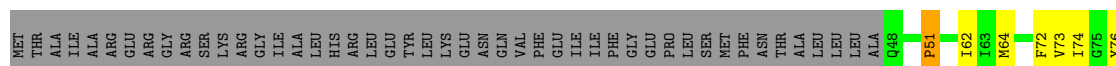
- Molecule 9: Photosystem I subunit III

Chain I:



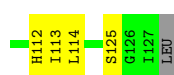
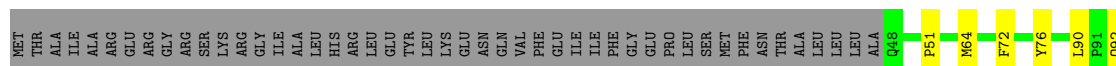
- Molecule 10: Photosystem I reaction center subunit VIII

Chain K:



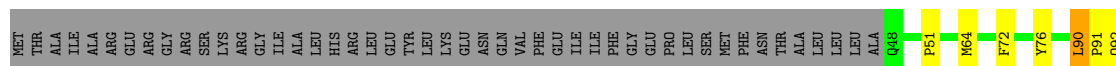
- Molecule 10: Photosystem I reaction center subunit VIII

Chain k:



- Molecule 10: Photosystem I reaction center subunit VIII

Chain 0:



4 Data and refinement statistics i

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	214.62Å 133.68Å 219.85Å 90.00° 111.14° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80	Depositor
% Data completeness (in resolution range)	95.4 (30.00-3.80)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4.1496)	Depositor
R, R_{free}	0.253 , 0.297	Depositor
Wilson B-factor (Å ²)	97.0	Xtriage
Anisotropy	0.297	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 153410 reflections	Xtriage
Total number of atoms	68370	wwPDB-VP
Average B, all atoms (Å ²)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.22	0/5970	0.37	0/8138
1	A	0.23	0/5970	0.38	0/8138
1	a	0.22	0/5970	0.37	0/8138
2	2	0.23	0/5976	0.39	0/8173
2	B	0.24	0/5976	0.39	0/8173
2	b	0.23	0/5976	0.38	0/8173
3	3	0.28	0/610	0.44	0/826
3	C	0.24	0/610	0.46	0/826
3	c	0.25	0/610	0.43	0/826
4	4	0.23	0/1103	0.40	0/1487
4	D	0.23	0/1103	0.40	0/1487
4	d	0.23	0/1103	0.39	0/1487
5	5	0.23	0/538	0.45	0/729
5	E	0.24	0/538	0.43	0/729
5	e	0.23	0/538	0.42	0/729
6	6	0.23	0/700	0.43	0/976
6	F	0.24	0/690	0.47	0/963
6	f	0.23	0/700	0.43	0/976
7	8	0.23	0/1163	0.38	0/1580
7	L	0.23	0/1163	0.38	0/1580
7	l	0.23	0/1163	0.38	0/1580
8	7	0.26	0/238	0.38	0/323
8	M	0.26	0/238	0.39	0/323
8	m	0.25	0/238	0.38	0/323
9	9	0.25	0/308	0.42	0/421
9	I	0.24	0/308	0.41	0/421
9	i	0.25	0/308	0.43	0/421
10	0	0.22	0/504	0.48	0/688
10	K	0.24	0/504	0.45	0/688
10	k	0.23	0/504	0.45	0/688
All	All	0.23	0/51320	0.39	0/70010

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
2	B	0	1
2	b	0	1
4	4	0	1
4	D	0	1
4	d	0	1
6	F	0	1
10	k	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	5	PHE	Peptide
4	D	98	HIS	Peptide
6	F	40	PRO	Mainchain
2	b	5	PHE	Peptide
4	d	98	HIS	Peptide

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	1	5772	0	5621	48	0
1	A	5772	0	5621	94	0
1	a	5772	0	5621	0	0
2	2	5765	0	5546	48	0
2	B	5765	0	5546	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	5765	0	5545	0	0
3	3	600	0	588	22	0
3	C	600	0	586	25	0
3	c	600	0	587	0	0
4	4	1079	0	1073	5	0
4	D	1079	0	1073	9	0
4	d	1079	0	1073	0	0
5	5	529	0	506	4	0
5	E	529	0	506	2	0
5	e	529	0	506	0	0
6	6	685	0	411	3	0
6	F	676	0	395	11	0
6	f	685	0	411	0	0
7	8	1133	0	1108	5	0
7	L	1133	0	1108	9	0
7	l	1133	0	1108	0	0
8	7	235	0	253	7	0
8	M	235	0	253	7	0
8	m	235	0	253	0	0
9	9	297	0	295	10	0
9	I	297	0	295	7	0
9	i	297	0	295	0	0
10	0	496	0	439	4	0
10	K	496	0	439	12	0
10	k	496	0	439	0	0
11	0	115	0	111	4	0
11	1	2546	0	2430	89	0
11	2	2313	0	2213	84	0
11	8	176	0	177	8	0
11	A	2546	0	2435	159	0
11	B	2313	0	2213	127	0
11	K	115	0	111	8	0
11	L	176	0	177	8	0
11	a	2546	0	2434	0	0
11	b	2313	0	2213	0	0
11	k	115	0	111	0	0
11	l	176	0	177	0	0
12	1	33	0	45	1	0
12	2	33	0	45	3	0
12	A	33	0	45	5	0
12	B	33	0	45	4	0
12	a	33	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	b	33	0	45	0	0
13	1	8	0	0	1	0
13	3	16	0	0	21	0
13	A	8	0	0	4	0
13	C	16	0	0	22	0
13	a	8	0	0	0	0
13	c	16	0	0	0	0
14	1	200	0	242	23	0
14	2	320	0	391	40	0
14	6	120	0	147	20	0
14	7	40	0	49	6	0
14	8	80	0	97	15	0
14	A	200	0	244	35	0
14	B	320	0	390	62	0
14	F	120	0	146	23	0
14	L	80	0	97	22	0
14	M	40	0	49	7	0
14	a	200	0	243	0	0
14	b	320	0	389	0	0
14	f	120	0	147	0	0
14	l	80	0	97	0	0
14	m	40	0	49	0	0
15	1	98	0	148	16	0
15	2	49	0	74	7	0
15	A	98	0	148	15	0
15	B	49	0	74	8	0
15	a	98	0	148	0	0
15	b	49	0	74	0	0
16	2	55	0	86	1	0
16	B	55	0	86	1	0
16	b	55	0	86	0	0
All	All	68370	0	66274	831	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 6.

The worst 5 of 831 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:48:CYS:SG	13:C:3002:SF4:FE4	0.75	1.74
3:3:48:CYS:SG	13:3:3002:SF4:FE4	0.87	1.64
1:A:56:HIS:CG	11:A:1103:CLA:HBB2	3.55	1.62
3:3:11:CYS:SG	13:3:3003:SF4:FE3	0.88	1.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:58:CYS:SG	13:C:3003:SF4:FE1	1.08	1.57

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	737/751 (98%)	697 (95%)	38 (5%)	2 (0%)	50	91
1	A	737/751 (98%)	693 (94%)	42 (6%)	2 (0%)	50	91
1	a	737/751 (98%)	698 (95%)	37 (5%)	2 (0%)	50	91
2	2	726/731 (99%)	691 (95%)	28 (4%)	7 (1%)	22	80
2	B	726/731 (99%)	690 (95%)	30 (4%)	6 (1%)	27	83
2	b	726/731 (99%)	692 (95%)	28 (4%)	6 (1%)	27	83
3	3	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	4	136/141 (96%)	121 (89%)	14 (10%)	1 (1%)	30	84
4	D	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	30	84
4	d	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	30	84
5	5	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	15	73
5	E	66/74 (89%)	57 (86%)	8 (12%)	1 (2%)	15	73
5	e	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	15	73
6	6	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	14	72
6	F	123/125 (98%)	114 (93%)	6 (5%)	3 (2%)	9	64
6	f	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	14	72
7	8	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	18	76
7	L	149/157 (95%)	135 (91%)	11 (7%)	3 (2%)	11	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	l	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	18	76
8	7	29/31 (94%)	29 (100%)	0	0	100	100
8	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
8	m	29/31 (94%)	29 (100%)	0	0	100	100
9	9	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	I	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	i	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
10	0	78/128 (61%)	65 (83%)	9 (12%)	4 (5%)	3	43
10	K	78/128 (61%)	66 (85%)	7 (9%)	5 (6%)	2	37
10	k	78/128 (61%)	66 (85%)	9 (12%)	3 (4%)	5	53
All	All	6474/6777 (96%)	6056 (94%)	361 (6%)	57 (1%)	25	81

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	THR
2	B	6	PRO
4	D	99	PRO
6	F	43	CYS
1	a	261	THR

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	588/603 (98%)	573 (97%)	15 (3%)	59	90
1	A	588/603 (98%)	570 (97%)	18 (3%)	52	89
1	a	588/603 (98%)	573 (97%)	15 (3%)	59	90
2	2	582/583 (100%)	565 (97%)	17 (3%)	55	89
2	B	582/583 (100%)	562 (97%)	20 (3%)	49	88
2	b	582/583 (100%)	566 (97%)	16 (3%)	57	90
3	3	68/69 (99%)	65 (96%)	3 (4%)	39	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	68/69 (99%)	61 (90%)	7 (10%)	10	51
3	c	68/69 (99%)	64 (94%)	4 (6%)	28	76
4	4	113/116 (97%)	109 (96%)	4 (4%)	48	88
4	D	113/116 (97%)	111 (98%)	2 (2%)	71	93
4	d	113/116 (97%)	110 (97%)	3 (3%)	57	90
5	5	56/60 (93%)	54 (96%)	2 (4%)	47	87
5	E	56/60 (93%)	54 (96%)	2 (4%)	47	87
5	e	56/60 (93%)	54 (96%)	2 (4%)	47	87
6	6	21/106 (20%)	20 (95%)	1 (5%)	35	82
6	F	19/106 (18%)	19 (100%)	0	100	100
6	f	21/106 (20%)	20 (95%)	1 (5%)	35	82
7	8	113/118 (96%)	113 (100%)	0	100	100
7	L	113/118 (96%)	112 (99%)	1 (1%)	87	97
7	l	113/118 (96%)	112 (99%)	1 (1%)	87	97
8	7	24/25 (96%)	23 (96%)	1 (4%)	40	84
8	M	24/25 (96%)	23 (96%)	1 (4%)	40	84
8	m	24/25 (96%)	23 (96%)	1 (4%)	40	84
9	9	31/32 (97%)	28 (90%)	3 (10%)	12	54
9	I	31/32 (97%)	27 (87%)	4 (13%)	6	39
9	i	31/32 (97%)	27 (87%)	4 (13%)	6	39
10	0	37/100 (37%)	30 (81%)	7 (19%)	2	17
10	K	37/100 (37%)	30 (81%)	7 (19%)	2	17
10	k	37/100 (37%)	31 (84%)	6 (16%)	3	26
All	All	4897/5436 (90%)	4729 (97%)	168 (3%)	49	88

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	334	LEU
9	i	21	LEU
10	k	64	MET
2	b	516	VAL
3	c	69	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	34	HIS
1	1	76	HIS
2	2	437	HIS
2	b	437	HIS
2	b	582	ASN

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 ⓘ

357 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	$\# Z > 2$
11	CLA	0	1401	-	73,73,73	2.19	20 (27%)	96,113,113	2.39	26 (27%)
11	CLA	0	1402	-	58,58,73	2.53	22 (37%)	76,95,113	2.50	23 (30%)
11	CLA	1	1011	-	73,73,73	2.16	19 (26%)	96,113,113	2.66	29 (30%)
11	CLA	1	1012	-	73,73,73	2.19	20 (27%)	96,113,113	2.45	29 (30%)
11	CLA	1	1022	-	73,73,73	2.19	20 (27%)	96,113,113	2.35	27 (28%)
11	CLA	1	1101	-	73,73,73	2.17	20 (27%)	96,113,113	2.30	27 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1102	-	73,73,73	2.21	21 (28%)	96,113,113	2.30	24 (25%)
11	CLA	1	1103	-	73,73,73	2.19	20 (27%)	96,113,113	2.37	27 (28%)
11	CLA	1	1104	-	73,73,73	2.21	19 (26%)	96,113,113	2.34	27 (28%)
11	CLA	1	1105	-	55,56,73	2.53	20 (36%)	74,92,113	2.55	23 (31%)
11	CLA	1	1106	1	73,73,73	2.23	21 (28%)	96,113,113	2.28	22 (22%)
11	CLA	1	1107	-	73,73,73	2.22	21 (28%)	96,113,113	2.33	23 (23%)
11	CLA	1	1108	-	51,53,73	2.59	20 (39%)	69,89,113	2.44	20 (28%)
11	CLA	1	1109	-	73,73,73	2.20	21 (28%)	96,113,113	2.33	26 (27%)
11	CLA	1	1110	-	62,62,73	2.39	20 (32%)	81,99,113	2.53	26 (32%)
11	CLA	1	1111	-	67,68,73	2.28	20 (29%)	88,107,113	2.50	28 (31%)
11	CLA	1	1112	-	51,53,73	2.60	20 (39%)	69,89,113	2.44	21 (30%)
11	CLA	1	1113	-	51,53,73	2.58	20 (39%)	69,89,113	2.40	18 (26%)
11	CLA	1	1114	-	53,54,73	2.52	19 (35%)	72,90,113	2.51	21 (29%)
11	CLA	1	1115	-	53,54,73	2.49	20 (37%)	72,90,113	2.63	23 (31%)
11	CLA	1	1116	-	62,62,73	2.40	20 (32%)	81,99,113	2.48	27 (33%)
11	CLA	1	1117	-	73,73,73	2.20	21 (28%)	96,113,113	2.28	27 (28%)
11	CLA	1	1118	-	69,69,73	2.35	20 (28%)	90,108,113	2.30	27 (30%)
11	CLA	1	1119	-	73,73,73	2.20	20 (27%)	96,113,113	2.31	27 (28%)
11	CLA	1	1120	-	53,54,73	2.51	19 (35%)	72,90,113	2.60	25 (34%)
11	CLA	1	1121	-	53,54,73	2.51	19 (35%)	72,90,113	2.57	21 (29%)
11	CLA	1	1122	-	67,67,73	2.31	19 (28%)	87,105,113	2.43	26 (29%)
11	CLA	1	1123	-	73,73,73	2.19	20 (27%)	96,113,113	2.31	26 (27%)
11	CLA	1	1124	-	62,63,73	2.39	20 (32%)	82,101,113	2.53	28 (34%)
11	CLA	1	1125	-	60,60,73	2.52	22 (36%)	80,97,113	2.56	29 (36%)
11	CLA	1	1126	-	73,73,73	2.21	21 (28%)	96,113,113	2.37	28 (29%)
11	CLA	1	1127	-	73,73,73	2.22	20 (27%)	96,113,113	2.25	25 (26%)
11	CLA	1	1128	-	73,73,73	2.20	21 (28%)	96,113,113	2.21	24 (25%)
11	CLA	1	1129	-	53,54,73	2.52	19 (35%)	72,90,113	2.53	24 (33%)
11	CLA	1	1130	-	53,54,73	2.53	19 (35%)	72,90,113	2.50	22 (30%)
11	CLA	1	1131	-	73,73,73	2.19	20 (27%)	96,113,113	2.29	26 (27%)
11	CLA	1	1132	-	73,73,73	2.18	20 (27%)	96,113,113	2.27	26 (27%)
11	CLA	1	1133	-	53,54,73	2.51	20 (37%)	72,90,113	2.52	24 (33%)
11	CLA	1	1134	-	53,54,73	2.52	19 (35%)	72,90,113	2.56	26 (36%)
11	CLA	1	1135	-	59,59,73	2.55	21 (35%)	78,96,113	2.56	29 (37%)
11	CLA	1	1136	-	53,54,73	2.50	19 (35%)	72,90,113	2.49	20 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1137	-	73,73,73	2.20	19 (26%)	96,113,113	2.46	30 (31%)
11	CLA	1	1138	-	53,54,73	2.49	19 (35%)	72,90,113	2.48	23 (31%)
11	CLA	1	1139	-	58,58,73	2.50	22 (37%)	76,95,113	2.53	25 (32%)
11	CLA	1	1140	-	73,73,73	2.20	21 (28%)	96,113,113	2.42	30 (31%)
11	CLA	1	1237	-	62,63,73	2.36	20 (32%)	82,101,113	2.46	29 (35%)
11	CLA	1	1801	15	60,60,73	2.55	22 (36%)	80,97,113	2.56	30 (37%)
12	PQN	1	2001	-	34,34,34	1.44	2 (5%)	45,45,45	1.01	2 (4%)
13	SF4	1	3001	1,2	12,12,12	6.50	12 (100%)	0,24,24	0.00	-
14	BCR	1	4001	-	41,41,41	2.71	6 (14%)	56,56,56	6.32	27 (48%)
14	BCR	1	4002	-	41,41,41	2.70	6 (14%)	56,56,56	6.73	24 (42%)
14	BCR	1	4003	-	41,41,41	2.76	6 (14%)	56,56,56	6.16	28 (50%)
14	BCR	1	4007	-	41,41,41	2.69	6 (14%)	56,56,56	6.44	25 (44%)
14	BCR	1	4008	-	41,41,41	2.70	6 (14%)	56,56,56	6.58	29 (51%)
15	LHG	1	5001	-	48,48,48	0.91	2 (4%)	54,54,54	1.06	3 (5%)
15	LHG	1	5003	11	48,48,48	0.91	2 (4%)	54,54,54	1.02	3 (5%)
11	CLA	2	1013	-	73,73,73	2.21	20 (27%)	96,113,113	2.40	30 (31%)
11	CLA	2	1021	-	73,73,73	2.19	20 (27%)	96,113,113	2.43	32 (33%)
11	CLA	2	1023	-	73,73,73	2.17	21 (28%)	96,113,113	2.52	33 (34%)
11	CLA	2	1201	-	62,62,73	2.40	20 (32%)	81,99,113	2.43	25 (30%)
11	CLA	2	1202	-	73,73,73	2.22	19 (26%)	96,113,113	2.33	25 (26%)
11	CLA	2	1203	-	73,73,73	2.16	19 (26%)	96,113,113	2.33	26 (27%)
11	CLA	2	1204	-	73,73,73	2.21	19 (26%)	96,113,113	2.27	27 (28%)
11	CLA	2	1205	-	62,63,73	2.36	19 (30%)	82,101,113	2.42	21 (25%)
11	CLA	2	1206	2	73,73,73	2.15	21 (28%)	96,113,113	2.25	24 (25%)
11	CLA	2	1207	-	73,73,73	2.17	20 (27%)	96,113,113	2.35	28 (29%)
11	CLA	2	1208	-	51,53,73	2.58	20 (39%)	69,89,113	2.38	17 (24%)
11	CLA	2	1209	-	51,53,73	2.58	20 (39%)	69,89,113	2.45	23 (33%)
11	CLA	2	1210	-	73,73,73	2.17	20 (27%)	96,113,113	2.36	31 (32%)
11	CLA	2	1211	-	53,54,73	2.50	18 (33%)	72,90,113	2.52	22 (30%)
11	CLA	2	1212	-	51,53,73	2.60	21 (41%)	69,89,113	2.42	21 (30%)
11	CLA	2	1213	-	73,73,73	2.26	21 (28%)	96,113,113	2.44	25 (26%)
11	CLA	2	1214	-	67,67,73	2.29	21 (31%)	87,105,113	2.40	27 (31%)
11	CLA	2	1215	-	73,73,73	2.20	20 (27%)	96,113,113	2.45	28 (29%)
11	CLA	2	1216	-	73,73,73	2.19	20 (27%)	96,113,113	2.29	30 (31%)
11	CLA	2	1217	-	54,55,73	2.88	20 (37%)	73,91,113	2.67	27 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	2	1218	-	51,53,73	2.59	20 (39%)	69,89,113	2.42	21 (30%)
11	CLA	2	1219	-	62,63,73	2.46	20 (32%)	82,101,113	2.57	30 (36%)
11	CLA	2	1220	-	53,54,73	2.50	19 (35%)	72,90,113	2.54	24 (33%)
11	CLA	2	1221	-	62,62,73	2.37	19 (30%)	81,99,113	2.55	28 (34%)
11	CLA	2	1222	-	64,64,73	2.45	20 (31%)	84,102,113	2.56	30 (35%)
11	CLA	2	1223	-	73,73,73	2.23	20 (27%)	96,113,113	2.31	27 (28%)
11	CLA	2	1224	-	62,63,73	2.36	20 (32%)	82,101,113	2.59	29 (35%)
11	CLA	2	1225	-	73,73,73	2.20	21 (28%)	96,113,113	2.28	26 (27%)
11	CLA	2	1226	-	73,73,73	2.21	20 (27%)	96,113,113	2.29	24 (25%)
11	CLA	2	1227	-	51,53,73	2.56	21 (41%)	69,89,113	2.46	19 (27%)
11	CLA	2	1228	-	58,58,73	2.48	21 (36%)	76,95,113	2.56	26 (34%)
11	CLA	2	1229	-	73,73,73	2.19	21 (28%)	96,113,113	2.29	27 (28%)
11	CLA	2	1230	-	65,66,73	2.34	21 (32%)	86,104,113	2.54	28 (32%)
11	CLA	2	1231	-	51,53,73	2.61	20 (39%)	69,89,113	2.54	24 (34%)
11	CLA	2	1232	-	51,53,73	2.58	20 (39%)	69,89,113	2.42	20 (28%)
11	CLA	2	1234	-	67,68,73	2.26	20 (29%)	88,107,113	2.47	23 (26%)
11	CLA	2	1235	-	67,68,73	2.30	19 (28%)	88,107,113	2.44	30 (34%)
11	CLA	2	1236	-	54,55,73	2.87	20 (37%)	73,91,113	2.59	22 (30%)
11	CLA	2	1238	-	73,73,73	2.20	21 (28%)	96,113,113	2.26	24 (25%)
11	CLA	2	1239	-	53,54,73	2.54	19 (35%)	72,90,113	2.55	22 (30%)
11	CLA	2	1240	15	51,53,73	2.60	21 (41%)	69,89,113	2.40	21 (30%)
12	PQN	2	2002	-	34,34,34	1.42	2 (5%)	45,45,45	1.00	5 (11%)
14	BCR	2	4004	-	41,41,41	2.69	6 (14%)	56,56,56	6.24	29 (51%)
14	BCR	2	4005	-	41,41,41	2.71	6 (14%)	56,56,56	6.16	21 (37%)
14	BCR	2	4006	-	41,41,41	2.70	6 (14%)	56,56,56	6.60	28 (50%)
14	BCR	2	4009	-	41,41,41	2.70	6 (14%)	56,56,56	6.53	25 (44%)
14	BCR	2	4010	-	41,41,41	2.82	6 (14%)	56,56,56	6.16	27 (48%)
14	BCR	2	4011	-	41,41,41	2.78	6 (14%)	56,56,56	6.55	26 (46%)
14	BCR	2	4014	-	41,41,41	2.78	6 (14%)	56,56,56	6.21	23 (41%)
14	BCR	2	4017	-	41,41,41	2.76	7 (17%)	56,56,56	6.30	29 (51%)
16	LMG	2	5002	-	55,55,55	0.87	2 (3%)	63,63,63	1.07	4 (6%)
15	LHG	2	5004	11	48,48,48	0.91	2 (4%)	54,54,54	1.04	3 (5%)
13	SF4	3	3002	3	12,12,12	6.42	12 (100%)	0,24,24	0.00	-
13	SF4	3	3003	-	12,12,12	6.54	12 (100%)	0,24,24	0.00	-
14	BCR	6	4013	-	41,41,41	2.67	6 (14%)	56,56,56	6.42	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	6	4018	-	41,41,41	2.85	7 (17%)	56,56,56	6.09	27 (48%)
14	BCR	6	4020	-	41,41,41	2.84	7 (17%)	56,56,56	6.31	23 (41%)
14	BCR	7	4021	-	41,41,41	2.76	6 (14%)	56,56,56	6.38	21 (37%)
11	CLA	8	1501	-	73,73,73	2.17	21 (28%)	96,113,113	2.37	28 (29%)
11	CLA	8	1502	-	53,54,73	2.48	19 (35%)	72,90,113	2.62	26 (36%)
11	CLA	8	1503	-	73,73,73	2.25	20 (27%)	96,113,113	2.31	23 (23%)
14	BCR	8	4019	-	41,41,41	2.73	6 (14%)	56,56,56	6.42	23 (41%)
14	BCR	8	4022	-	41,41,41	2.77	6 (14%)	56,56,56	6.27	29 (51%)
11	CLA	A	1011	-	73,73,73	2.19	19 (26%)	96,113,113	2.41	28 (29%)
11	CLA	A	1012	-	73,73,73	2.19	21 (28%)	96,113,113	2.53	32 (33%)
11	CLA	A	1022	-	73,73,73	2.19	20 (27%)	96,113,113	2.37	27 (28%)
11	CLA	A	1101	-	73,73,73	2.19	20 (27%)	96,113,113	2.28	26 (27%)
11	CLA	A	1102	11	73,73,73	2.21	20 (27%)	96,113,113	2.34	28 (29%)
11	CLA	A	1103	-	73,73,73	2.22	19 (26%)	96,113,113	2.31	28 (29%)
11	CLA	A	1104	-	73,73,73	2.17	19 (26%)	96,113,113	2.40	29 (30%)
11	CLA	A	1105	-	55,56,73	2.52	19 (34%)	74,92,113	2.52	24 (32%)
11	CLA	A	1106	1	73,73,73	2.19	21 (28%)	96,113,113	2.32	25 (26%)
11	CLA	A	1107	1	73,73,73	2.18	19 (26%)	96,113,113	2.40	29 (30%)
11	CLA	A	1108	-	51,53,73	2.59	20 (39%)	69,89,113	2.45	20 (28%)
11	CLA	A	1109	11	73,73,73	2.23	20 (27%)	96,113,113	2.34	26 (27%)
11	CLA	A	1110	-	62,62,73	2.42	21 (33%)	81,99,113	2.50	25 (30%)
11	CLA	A	1111	-	67,68,73	2.27	20 (29%)	88,107,113	2.41	28 (31%)
11	CLA	A	1112	-	51,53,73	2.61	21 (41%)	69,89,113	2.52	23 (33%)
11	CLA	A	1113	-	51,53,73	2.58	19 (37%)	69,89,113	2.47	21 (30%)
11	CLA	A	1114	-	53,54,73	2.51	20 (37%)	72,90,113	2.46	21 (29%)
11	CLA	A	1115	-	53,54,73	2.55	20 (37%)	72,90,113	2.54	21 (29%)
11	CLA	A	1116	-	62,62,73	2.39	21 (33%)	81,99,113	2.51	27 (33%)
11	CLA	A	1117	-	73,73,73	2.26	21 (28%)	96,113,113	2.36	27 (28%)
11	CLA	A	1118	-	69,69,73	2.33	21 (30%)	90,108,113	2.32	24 (26%)
11	CLA	A	1119	-	73,73,73	2.18	22 (30%)	96,113,113	2.28	28 (29%)
11	CLA	A	1120	-	53,54,73	2.51	19 (35%)	72,90,113	2.60	24 (33%)
11	CLA	A	1121	-	53,54,73	2.54	19 (35%)	72,90,113	2.52	22 (30%)
11	CLA	A	1122	-	67,67,73	2.30	21 (31%)	87,105,113	2.51	28 (32%)
11	CLA	A	1123	-	73,73,73	2.15	21 (28%)	96,113,113	2.34	29 (30%)
11	CLA	A	1124	-	62,63,73	2.38	21 (33%)	82,101,113	2.57	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	1125	-	60,60,73	2.51	22 (36%)	80,97,113	2.64	27 (33%)
11	CLA	A	1126	-	73,73,73	2.22	20 (27%)	96,113,113	2.40	30 (31%)
11	CLA	A	1127	-	73,73,73	2.18	20 (27%)	96,113,113	2.36	28 (29%)
11	CLA	A	1128	-	73,73,73	2.19	20 (27%)	96,113,113	2.21	24 (25%)
11	CLA	A	1129	-	53,54,73	2.51	20 (37%)	72,90,113	2.48	23 (31%)
11	CLA	A	1130	-	53,54,73	2.50	18 (33%)	72,90,113	2.51	22 (30%)
11	CLA	A	1131	-	73,73,73	2.19	20 (27%)	96,113,113	2.28	27 (28%)
11	CLA	A	1132	-	73,73,73	2.20	20 (27%)	96,113,113	2.35	26 (27%)
11	CLA	A	1133	-	53,54,73	2.45	20 (37%)	72,90,113	2.57	25 (34%)
11	CLA	A	1134	1	53,54,73	2.50	19 (35%)	72,90,113	2.54	27 (37%)
11	CLA	A	1135	-	59,59,73	2.53	22 (37%)	78,96,113	2.61	28 (35%)
11	CLA	A	1136	-	53,54,73	2.50	21 (39%)	72,90,113	2.50	20 (27%)
11	CLA	A	1137	-	73,73,73	2.24	21 (28%)	96,113,113	2.50	30 (31%)
11	CLA	A	1138	-	53,54,73	2.48	20 (37%)	72,90,113	2.56	24 (33%)
11	CLA	A	1139	-	58,58,73	2.49	21 (36%)	76,95,113	2.53	25 (32%)
11	CLA	A	1140	-	73,73,73	2.21	21 (28%)	96,113,113	2.34	26 (27%)
11	CLA	A	1237	-	62,63,73	2.38	20 (32%)	82,101,113	2.48	25 (30%)
11	CLA	A	1801	15	60,60,73	2.57	22 (36%)	80,97,113	2.58	25 (31%)
12	PQN	A	2001	-	34,34,34	1.43	2 (5%)	45,45,45	1.05	5 (11%)
13	SF4	A	3001	1,2	12,12,12	6.47	12 (100%)	0,24,24	0.00	-
14	BCR	A	4001	-	41,41,41	2.76	6 (14%)	56,56,56	6.17	26 (46%)
14	BCR	A	4002	-	41,41,41	2.72	6 (14%)	56,56,56	6.10	24 (42%)
14	BCR	A	4003	-	41,41,41	2.83	6 (14%)	56,56,56	6.06	24 (42%)
14	BCR	A	4007	-	41,41,41	2.74	6 (14%)	56,56,56	6.58	22 (39%)
14	BCR	A	4008	-	41,41,41	2.70	6 (14%)	56,56,56	6.47	29 (51%)
15	LHG	A	5001	-	48,48,48	0.89	2 (4%)	54,54,54	1.10	3 (5%)
15	LHG	A	5003	11	48,48,48	0.91	2 (4%)	54,54,54	1.12	4 (7%)
11	CLA	B	1013	-	73,73,73	2.19	20 (27%)	96,113,113	2.37	29 (30%)
11	CLA	B	1021	-	73,73,73	2.17	20 (27%)	96,113,113	2.42	28 (29%)
11	CLA	B	1023	-	73,73,73	2.16	20 (27%)	96,113,113	2.43	30 (31%)
11	CLA	B	1201	-	62,62,73	2.38	21 (33%)	81,99,113	2.52	28 (34%)
11	CLA	B	1202	-	73,73,73	2.26	20 (27%)	96,113,113	2.38	26 (27%)
11	CLA	B	1203	-	73,73,73	2.19	20 (27%)	96,113,113	2.30	25 (26%)
11	CLA	B	1204	-	73,73,73	2.17	19 (26%)	96,113,113	2.30	26 (27%)
11	CLA	B	1205	-	62,63,73	2.33	20 (32%)	82,101,113	2.53	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	1206	2	73,73,73	2.15	21 (28%)	96,113,113	2.26	27 (28%)
11	CLA	B	1207	-	73,73,73	2.17	20 (27%)	96,113,113	2.36	24 (25%)
11	CLA	B	1208	-	51,53,73	2.61	20 (39%)	69,89,113	2.39	18 (26%)
11	CLA	B	1209	-	51,53,73	2.58	20 (39%)	69,89,113	2.46	25 (36%)
11	CLA	B	1210	-	73,73,73	2.20	21 (28%)	96,113,113	2.32	29 (30%)
11	CLA	B	1211	-	53,54,73	2.48	19 (35%)	72,90,113	2.49	22 (30%)
11	CLA	B	1212	-	51,53,73	2.59	20 (39%)	69,89,113	2.45	20 (28%)
11	CLA	B	1213	-	73,73,73	2.21	20 (27%)	96,113,113	2.28	26 (27%)
11	CLA	B	1214	-	67,67,73	2.30	20 (29%)	87,105,113	2.56	34 (39%)
11	CLA	B	1215	-	73,73,73	2.19	20 (27%)	96,113,113	2.48	29 (30%)
11	CLA	B	1216	-	73,73,73	2.19	21 (28%)	96,113,113	2.31	27 (28%)
11	CLA	B	1217	-	54,55,73	2.90	19 (35%)	73,91,113	2.61	25 (34%)
11	CLA	B	1218	-	51,53,73	2.58	21 (41%)	69,89,113	2.43	20 (28%)
11	CLA	B	1219	-	62,63,73	2.39	20 (32%)	82,101,113	2.45	27 (32%)
11	CLA	B	1220	-	53,54,73	2.48	19 (35%)	72,90,113	2.50	22 (30%)
11	CLA	B	1221	-	62,62,73	2.36	19 (30%)	81,99,113	2.51	27 (33%)
11	CLA	B	1222	-	64,64,73	2.51	21 (32%)	84,102,113	2.74	34 (40%)
11	CLA	B	1223	-	73,73,73	2.21	21 (28%)	96,113,113	2.33	27 (28%)
11	CLA	B	1224	-	62,63,73	2.38	19 (30%)	82,101,113	2.59	28 (34%)
11	CLA	B	1225	-	73,73,73	2.19	20 (27%)	96,113,113	2.25	25 (26%)
11	CLA	B	1226	-	73,73,73	2.17	19 (26%)	96,113,113	2.33	28 (29%)
11	CLA	B	1227	-	51,53,73	2.56	21 (41%)	69,89,113	2.48	22 (31%)
11	CLA	B	1228	-	58,58,73	2.49	22 (37%)	76,95,113	2.54	23 (30%)
11	CLA	B	1229	-	73,73,73	2.20	21 (28%)	96,113,113	2.29	26 (27%)
11	CLA	B	1230	-	65,66,73	2.32	21 (32%)	86,104,113	2.51	27 (31%)
11	CLA	B	1231	-	51,53,73	2.57	20 (39%)	69,89,113	2.53	24 (34%)
11	CLA	B	1232	-	51,53,73	2.55	20 (39%)	69,89,113	2.41	19 (27%)
11	CLA	B	1234	-	67,68,73	2.26	21 (31%)	88,107,113	2.47	26 (29%)
11	CLA	B	1235	-	67,68,73	2.31	20 (29%)	88,107,113	2.45	24 (27%)
11	CLA	B	1236	-	54,55,73	2.86	20 (37%)	73,91,113	2.67	23 (31%)
11	CLA	B	1238	-	73,73,73	2.17	19 (26%)	96,113,113	2.23	24 (25%)
11	CLA	B	1239	-	53,54,73	2.51	18 (33%)	72,90,113	2.54	22 (30%)
11	CLA	B	1240	15	51,53,73	2.63	21 (41%)	69,89,113	2.47	21 (30%)
12	PQN	B	2002	-	34,34,34	1.42	2 (5%)	45,45,45	1.05	5 (11%)
14	BCR	B	4004	-	41,41,41	2.78	6 (14%)	56,56,56	6.33	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	B	4005	-	41,41,41	2.77	6 (14%)	56,56,56	6.30	25 (44%)
14	BCR	B	4006	-	41,41,41	2.72	6 (14%)	56,56,56	6.59	27 (48%)
14	BCR	B	4009	-	41,41,41	2.73	6 (14%)	56,56,56	6.48	20 (35%)
14	BCR	B	4010	-	41,41,41	2.70	6 (14%)	56,56,56	6.18	26 (46%)
14	BCR	B	4011	-	41,41,41	2.79	7 (17%)	56,56,56	6.50	28 (50%)
14	BCR	B	4014	-	41,41,41	2.75	6 (14%)	56,56,56	6.07	25 (44%)
14	BCR	B	4017	-	41,41,41	2.75	6 (14%)	56,56,56	6.37	31 (55%)
16	LMG	B	5002	-	55,55,55	0.86	2 (3%)	63,63,63	1.08	4 (6%)
15	LHG	B	5004	11	48,48,48	0.91	2 (4%)	54,54,54	1.11	3 (5%)
13	SF4	C	3002	3	12,12,12	6.38	12 (100%)	0,24,24	0.00	-
13	SF4	C	3003	3	12,12,12	6.52	12 (100%)	0,24,24	0.00	-
14	BCR	F	4013	-	41,41,41	2.76	6 (14%)	56,56,56	6.56	20 (35%)
14	BCR	F	4018	-	41,41,41	2.89	7 (17%)	56,56,56	6.34	24 (42%)
14	BCR	F	4020	-	41,41,41	2.77	6 (14%)	56,56,56	6.17	23 (41%)
11	CLA	K	1401	-	73,73,73	2.19	20 (27%)	96,113,113	2.39	27 (28%)
11	CLA	K	1402	-	58,58,73	2.50	22 (37%)	76,95,113	2.49	24 (31%)
11	CLA	L	1501	7	73,73,73	2.19	19 (26%)	96,113,113	2.31	28 (29%)
11	CLA	L	1502	-	53,54,73	2.49	18 (33%)	72,90,113	2.57	23 (31%)
11	CLA	L	1503	-	73,73,73	2.17	19 (26%)	96,113,113	2.32	23 (23%)
14	BCR	L	4019	-	41,41,41	2.67	6 (14%)	56,56,56	6.35	26 (46%)
14	BCR	L	4022	-	41,41,41	2.67	6 (14%)	56,56,56	5.89	25 (44%)
14	BCR	M	4021	-	41,41,41	2.77	6 (14%)	56,56,56	6.34	21 (37%)
11	CLA	a	1011	-	73,73,73	2.22	21 (28%)	96,113,113	2.45	28 (29%)
11	CLA	a	1012	-	73,73,73	2.20	21 (28%)	96,113,113	2.41	28 (29%)
11	CLA	a	1022	-	73,73,73	2.18	20 (27%)	96,113,113	2.33	25 (26%)
11	CLA	a	1101	-	73,73,73	2.21	20 (27%)	96,113,113	2.35	28 (29%)
11	CLA	a	1102	11	73,73,73	2.20	20 (27%)	96,113,113	2.32	25 (26%)
11	CLA	a	1103	-	73,73,73	2.21	20 (27%)	96,113,113	2.33	25 (26%)
11	CLA	a	1104	-	73,73,73	2.18	20 (27%)	96,113,113	2.35	28 (29%)
11	CLA	a	1105	-	55,56,73	2.55	20 (36%)	74,92,113	2.61	24 (32%)
11	CLA	a	1106	1	73,73,73	2.22	21 (28%)	96,113,113	2.32	28 (29%)
11	CLA	a	1107	1	73,73,73	2.17	20 (27%)	96,113,113	2.46	27 (28%)
11	CLA	a	1108	-	51,53,73	2.60	20 (39%)	69,89,113	2.42	21 (30%)
11	CLA	a	1109	11	73,73,73	2.23	20 (27%)	96,113,113	2.37	28 (29%)
11	CLA	a	1110	-	62,62,73	2.42	21 (33%)	81,99,113	2.46	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	a	1111	-	67,68,73	2.28	19 (28%)	88,107,113	2.42	28 (31%)
11	CLA	a	1112	-	51,53,73	2.61	20 (39%)	69,89,113	2.42	19 (27%)
11	CLA	a	1113	-	51,53,73	2.59	20 (39%)	69,89,113	2.42	21 (30%)
11	CLA	a	1114	-	53,54,73	2.50	19 (35%)	72,90,113	2.50	23 (31%)
11	CLA	a	1115	-	53,54,73	2.54	20 (37%)	72,90,113	2.50	20 (27%)
11	CLA	a	1116	-	62,62,73	2.42	22 (35%)	81,99,113	2.50	25 (30%)
11	CLA	a	1117	-	73,73,73	2.22	20 (27%)	96,113,113	2.30	26 (27%)
11	CLA	a	1118	-	69,69,73	2.36	21 (30%)	90,108,113	2.33	23 (25%)
11	CLA	a	1119	-	73,73,73	2.19	22 (30%)	96,113,113	2.30	26 (27%)
11	CLA	a	1120	-	53,54,73	2.51	19 (35%)	72,90,113	2.61	23 (31%)
11	CLA	a	1121	-	53,54,73	2.50	19 (35%)	72,90,113	2.59	24 (33%)
11	CLA	a	1122	-	67,67,73	2.32	19 (28%)	87,105,113	2.48	28 (32%)
11	CLA	a	1123	-	73,73,73	2.20	20 (27%)	96,113,113	2.27	25 (26%)
11	CLA	a	1124	-	62,63,73	2.38	21 (33%)	82,101,113	2.59	29 (35%)
11	CLA	a	1125	-	60,60,73	2.53	21 (35%)	80,97,113	2.50	24 (30%)
11	CLA	a	1126	-	73,73,73	2.22	20 (27%)	96,113,113	2.36	28 (29%)
11	CLA	a	1127	-	73,73,73	2.21	21 (28%)	96,113,113	2.31	30 (31%)
11	CLA	a	1128	-	73,73,73	2.22	21 (28%)	96,113,113	2.27	25 (26%)
11	CLA	a	1129	-	53,54,73	2.51	18 (33%)	72,90,113	2.54	21 (29%)
11	CLA	a	1130	-	53,54,73	2.53	19 (35%)	72,90,113	2.57	24 (33%)
11	CLA	a	1131	-	73,73,73	2.20	20 (27%)	96,113,113	2.30	26 (27%)
11	CLA	a	1132	-	73,73,73	2.20	20 (27%)	96,113,113	2.34	28 (29%)
11	CLA	a	1133	-	53,54,73	2.49	20 (37%)	72,90,113	2.53	24 (33%)
11	CLA	a	1134	-	53,54,73	2.53	19 (35%)	72,90,113	2.57	26 (36%)
11	CLA	a	1135	-	59,59,73	2.52	22 (37%)	78,96,113	2.52	25 (32%)
11	CLA	a	1136	-	53,54,73	2.50	21 (39%)	72,90,113	2.52	22 (30%)
11	CLA	a	1137	-	73,73,73	2.20	20 (27%)	96,113,113	2.43	28 (29%)
11	CLA	a	1138	-	53,54,73	2.50	19 (35%)	72,90,113	2.59	28 (38%)
11	CLA	a	1139	-	58,58,73	2.48	21 (36%)	76,95,113	2.52	27 (35%)
11	CLA	a	1140	-	73,73,73	2.19	20 (27%)	96,113,113	2.30	27 (28%)
11	CLA	a	1237	-	62,63,73	2.40	20 (32%)	82,101,113	2.41	22 (26%)
11	CLA	a	1801	15	60,60,73	2.55	21 (35%)	80,97,113	2.57	26 (32%)
12	PQN	a	2001	-	34,34,34	1.42	2 (5%)	45,45,45	0.97	4 (8%)
13	SF4	a	3001	1,2	12,12,12	6.49	12 (100%)	0,24,24	0.00	-
14	BCR	a	4001	-	41,41,41	2.72	6 (14%)	56,56,56	6.29	27 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	a	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.37	26 (46%)
14	BCR	a	4003	-	41,41,41	2.73	6 (14%)	56,56,56	5.98	26 (46%)
14	BCR	a	4007	-	41,41,41	2.70	6 (14%)	56,56,56	6.51	23 (41%)
14	BCR	a	4008	-	41,41,41	2.72	7 (17%)	56,56,56	6.35	29 (51%)
15	LHG	a	5001	-	48,48,48	0.91	2 (4%)	54,54,54	1.05	3 (5%)
15	LHG	a	5003	11	48,48,48	0.90	2 (4%)	54,54,54	1.02	3 (5%)
11	CLA	b	1013	-	73,73,73	2.21	20 (27%)	96,113,113	2.36	28 (29%)
11	CLA	b	1021	-	73,73,73	2.22	20 (27%)	96,113,113	2.38	32 (33%)
11	CLA	b	1023	-	73,73,73	2.17	21 (28%)	96,113,113	2.42	29 (30%)
11	CLA	b	1201	-	62,62,73	2.42	19 (30%)	81,99,113	2.55	26 (32%)
11	CLA	b	1202	-	73,73,73	2.21	20 (27%)	96,113,113	2.33	27 (28%)
11	CLA	b	1203	-	73,73,73	2.19	21 (28%)	96,113,113	2.33	28 (29%)
11	CLA	b	1204	-	73,73,73	2.19	19 (26%)	96,113,113	2.25	23 (23%)
11	CLA	b	1205	-	62,63,73	2.35	20 (32%)	82,101,113	2.49	26 (31%)
11	CLA	b	1206	2	73,73,73	2.17	21 (28%)	96,113,113	2.26	28 (29%)
11	CLA	b	1207	-	73,73,73	2.17	21 (28%)	96,113,113	2.33	23 (23%)
11	CLA	b	1208	-	51,53,73	2.60	20 (39%)	69,89,113	2.43	19 (27%)
11	CLA	b	1209	-	51,53,73	2.61	21 (41%)	69,89,113	2.44	22 (31%)
11	CLA	b	1210	-	73,73,73	2.22	20 (27%)	96,113,113	2.32	29 (30%)
11	CLA	b	1211	-	53,54,73	2.51	19 (35%)	72,90,113	2.52	21 (29%)
11	CLA	b	1212	-	51,53,73	2.57	22 (43%)	69,89,113	2.43	17 (24%)
11	CLA	b	1213	-	73,73,73	2.23	21 (28%)	96,113,113	2.30	24 (25%)
11	CLA	b	1214	-	67,67,73	2.31	20 (29%)	87,105,113	2.44	30 (34%)
11	CLA	b	1215	-	73,73,73	2.21	20 (27%)	96,113,113	2.44	27 (28%)
11	CLA	b	1216	-	73,73,73	2.21	20 (27%)	96,113,113	2.28	30 (31%)
11	CLA	b	1217	-	54,55,73	2.88	20 (37%)	73,91,113	2.57	23 (31%)
11	CLA	b	1218	-	51,53,73	2.60	20 (39%)	69,89,113	2.42	19 (27%)
11	CLA	b	1219	-	62,63,73	2.42	20 (32%)	82,101,113	2.51	27 (32%)
11	CLA	b	1220	-	53,54,73	2.53	19 (35%)	72,90,113	2.53	25 (34%)
11	CLA	b	1221	-	62,62,73	2.39	20 (32%)	81,99,113	2.61	29 (35%)
11	CLA	b	1222	-	64,64,73	2.46	21 (32%)	84,102,113	2.64	31 (36%)
11	CLA	b	1223	-	73,73,73	2.25	20 (27%)	96,113,113	2.27	23 (23%)
11	CLA	b	1224	-	62,63,73	2.40	20 (32%)	82,101,113	2.53	28 (34%)
11	CLA	b	1225	-	73,73,73	2.20	20 (27%)	96,113,113	2.25	27 (28%)
11	CLA	b	1226	-	73,73,73	2.19	20 (27%)	96,113,113	2.27	26 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	b	1227	-	51,53,73	2.57	20 (39%)	69,89,113	2.49	20 (28%)
11	CLA	b	1228	-	58,58,73	2.49	21 (36%)	76,95,113	2.55	25 (32%)
11	CLA	b	1229	-	73,73,73	2.21	20 (27%)	96,113,113	2.27	25 (26%)
11	CLA	b	1230	-	65,66,73	2.35	21 (32%)	86,104,113	2.53	28 (32%)
11	CLA	b	1231	-	51,53,73	2.59	20 (39%)	69,89,113	2.48	22 (31%)
11	CLA	b	1232	-	51,53,73	2.59	20 (39%)	69,89,113	2.43	21 (30%)
11	CLA	b	1234	-	67,68,73	2.28	21 (31%)	88,107,113	2.39	26 (29%)
11	CLA	b	1235	-	67,68,73	2.33	20 (29%)	88,107,113	2.48	30 (34%)
11	CLA	b	1236	-	54,55,73	2.89	20 (37%)	73,91,113	2.62	24 (32%)
11	CLA	b	1238	-	73,73,73	2.20	22 (30%)	96,113,113	2.28	25 (26%)
11	CLA	b	1239	-	53,54,73	2.52	20 (37%)	72,90,113	2.55	22 (30%)
11	CLA	b	1240	-	51,53,73	2.61	20 (39%)	69,89,113	2.44	21 (30%)
12	PQN	b	2002	-	34,34,34	1.42	2 (5%)	45,45,45	1.02	4 (8%)
14	BCR	b	4004	-	41,41,41	2.72	6 (14%)	56,56,56	6.34	26 (46%)
14	BCR	b	4005	-	41,41,41	2.74	6 (14%)	56,56,56	6.35	24 (42%)
14	BCR	b	4006	-	41,41,41	2.74	6 (14%)	56,56,56	6.72	27 (48%)
14	BCR	b	4009	-	41,41,41	2.63	6 (14%)	56,56,56	6.70	26 (46%)
14	BCR	b	4010	-	41,41,41	2.77	6 (14%)	56,56,56	6.49	23 (41%)
14	BCR	b	4011	-	41,41,41	2.73	6 (14%)	56,56,56	6.57	25 (44%)
14	BCR	b	4014	-	41,41,41	2.72	6 (14%)	56,56,56	6.27	23 (41%)
14	BCR	b	4017	-	41,41,41	2.79	7 (17%)	56,56,56	6.44	28 (50%)
16	LMG	b	5002	-	55,55,55	0.85	2 (3%)	63,63,63	1.06	5 (7%)
15	LHG	b	5004	-	48,48,48	0.90	2 (4%)	54,54,54	1.03	3 (5%)
13	SF4	c	3002	3	12,12,12	6.42	12 (100%)	0,24,24	0.00	-
13	SF4	c	3003	3	12,12,12	6.52	12 (100%)	0,24,24	0.00	-
14	BCR	f	4013	-	41,41,41	2.73	6 (14%)	56,56,56	6.41	23 (41%)
14	BCR	f	4018	-	41,41,41	2.83	7 (17%)	56,56,56	6.14	24 (42%)
14	BCR	f	4020	-	41,41,41	2.77	6 (14%)	56,56,56	6.34	22 (39%)
11	CLA	k	1401	-	73,73,73	2.20	20 (27%)	96,113,113	2.40	27 (28%)
11	CLA	k	1402	-	58,58,73	2.53	23 (39%)	76,95,113	2.54	22 (28%)
11	CLA	l	1501	7	73,73,73	2.20	20 (27%)	96,113,113	2.33	29 (30%)
11	CLA	l	1502	-	53,54,73	2.50	18 (33%)	72,90,113	2.54	22 (30%)
11	CLA	l	1503	-	73,73,73	2.19	19 (26%)	96,113,113	2.30	23 (23%)
14	BCR	l	4019	-	41,41,41	2.73	6 (14%)	56,56,56	6.47	22 (39%)
14	BCR	l	4022	-	41,41,41	2.72	6 (14%)	56,56,56	6.18	27 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	m	4021	-	41,41,41	2.82	6 (14%)	56,56,56	6.27	24 (42%)

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
11	CLA	0	1401	-	-	0/37/135/135	0/0/9/9
11	CLA	0	1402	-	-	0/19/117/135	0/0/9/9
11	CLA	1	1011	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1012	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1022	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1101	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1102	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1103	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1104	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1105	-	-	0/17/115/135	0/0/9/9
11	CLA	1	1106	1	-	0/37/135/135	0/0/9/9
11	CLA	1	1107	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1108	-	-	0/11/111/135	0/0/9/9
11	CLA	1	1109	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1110	-	-	0/23/122/135	0/0/9/9
11	CLA	1	1111	-	-	0/31/129/135	0/0/9/9
11	CLA	1	1112	-	-	0/11/111/135	0/0/9/9
11	CLA	1	1113	-	-	0/11/111/135	0/0/9/9
11	CLA	1	1114	-	-	0/15/113/135	0/0/9/9
11	CLA	1	1115	-	-	0/15/113/135	0/0/9/9
11	CLA	1	1116	-	-	0/23/122/135	0/0/9/9
11	CLA	1	1117	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1118	-	-	0/33/131/135	0/0/9/9
11	CLA	1	1119	-	-	1/37/135/135	0/0/9/9
11	CLA	1	1120	-	-	0/15/113/135	0/0/9/9
11	CLA	1	1121	-	-	0/15/113/135	0/0/9/9
11	CLA	1	1122	-	-	0/29/128/135	0/0/9/9
11	CLA	1	1123	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1124	-	-	0/25/123/135	0/0/9/9
11	CLA	1	1125	-	-	0/22/120/135	0/0/9/9
11	CLA	1	1126	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1127	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1128	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1129	-	-	0/15/113/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	1	1130	-	-	0/15/113/135	0/0/9/9
11	CLA	1	1131	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1132	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1133	-	-	0/15/113/135	0/0/9/9
11	CLA	1	1134	-	-	0/15/113/135	0/0/9/9
11	CLA	1	1135	-	-	0/21/119/135	0/0/9/9
11	CLA	1	1136	-	-	0/15/113/135	0/0/9/9
11	CLA	1	1137	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1138	-	-	0/15/113/135	0/0/9/9
11	CLA	1	1139	-	-	0/19/117/135	0/0/9/9
11	CLA	1	1140	-	-	0/37/135/135	0/0/9/9
11	CLA	1	1237	-	-	0/25/123/135	0/0/9/9
11	CLA	1	1801	15	-	0/22/120/135	0/0/9/9
12	PQN	1	2001	-	-	0/23/43/43	0/2/2/2
13	SF4	1	3001	1,2	-	0/0/48/48	0/6/5/5
14	BCR	1	4001	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4002	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4003	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4007	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4008	-	-	1/29/63/63	0/2/2/2
15	LHG	1	5001	-	-	0/53/53/53	0/0/0/0
15	LHG	1	5003	11	-	0/53/53/53	0/0/0/0
11	CLA	2	1013	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1021	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1023	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1201	-	-	0/23/122/135	0/0/9/9
11	CLA	2	1202	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1203	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1204	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1205	-	-	0/25/123/135	0/0/9/9
11	CLA	2	1206	2	-	0/37/135/135	0/0/9/9
11	CLA	2	1207	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1208	-	-	0/11/111/135	0/0/9/9
11	CLA	2	1209	-	-	0/11/111/135	0/0/9/9
11	CLA	2	1210	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1211	-	-	0/15/113/135	0/0/9/9
11	CLA	2	1212	-	-	0/11/111/135	0/0/9/9
11	CLA	2	1213	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1214	-	-	0/29/128/135	0/0/9/9
11	CLA	2	1215	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1216	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1217	-	-	0/16/114/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	2	1218	-	-	0/11/111/135	0/0/9/9
11	CLA	2	1219	-	-	0/25/123/135	0/0/9/9
11	CLA	2	1220	-	-	0/15/113/135	0/0/9/9
11	CLA	2	1221	-	-	0/23/122/135	0/0/9/9
11	CLA	2	1222	-	-	0/27/125/135	0/0/9/9
11	CLA	2	1223	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1224	-	-	0/25/123/135	0/0/9/9
11	CLA	2	1225	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1226	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1227	-	-	0/11/111/135	0/0/9/9
11	CLA	2	1228	-	-	0/19/117/135	0/0/9/9
11	CLA	2	1229	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1230	-	-	0/29/127/135	0/0/9/9
11	CLA	2	1231	-	-	0/11/111/135	0/0/9/9
11	CLA	2	1232	-	-	0/11/111/135	0/0/9/9
11	CLA	2	1234	-	-	0/31/129/135	0/0/9/9
11	CLA	2	1235	-	-	0/31/129/135	0/0/9/9
11	CLA	2	1236	-	-	0/16/114/135	0/0/9/9
11	CLA	2	1238	-	-	0/37/135/135	0/0/9/9
11	CLA	2	1239	-	-	0/15/113/135	0/0/9/9
11	CLA	2	1240	15	-	0/11/111/135	0/0/9/9
12	PQN	2	2002	-	-	0/23/43/43	0/2/2/2
14	BCR	2	4004	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4005	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4006	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4009	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4010	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4011	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4014	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4017	-	-	2/29/63/63	0/2/2/2
16	LMG	2	5002	-	-	0/50/70/70	0/1/1/1
15	LHG	2	5004	11	-	0/53/53/53	0/0/0/0
13	SF4	3	3002	3	-	0/0/48/48	0/6/5/5
13	SF4	3	3003	-	-	0/0/48/48	0/6/5/5
14	BCR	6	4013	-	-	0/29/63/63	0/2/2/2
14	BCR	6	4018	-	-	0/29/63/63	0/2/2/2
14	BCR	6	4020	-	-	1/29/63/63	0/2/2/2
14	BCR	7	4021	-	-	0/29/63/63	0/2/2/2
11	CLA	8	1501	-	-	0/37/135/135	0/0/9/9
11	CLA	8	1502	-	-	0/15/113/135	0/0/9/9
11	CLA	8	1503	-	-	0/37/135/135	0/0/9/9
14	BCR	8	4019	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	8	4022	-	-	0/29/63/63	0/2/2/2
11	CLA	A	1011	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1012	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1022	-	-	1/37/135/135	0/0/9/9
11	CLA	A	1101	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1102	11	-	0/37/135/135	0/0/9/9
11	CLA	A	1103	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1104	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1105	-	-	0/17/115/135	0/0/9/9
11	CLA	A	1106	1	-	0/37/135/135	0/0/9/9
11	CLA	A	1107	1	-	0/37/135/135	0/0/9/9
11	CLA	A	1108	-	-	0/11/111/135	0/0/9/9
11	CLA	A	1109	11	-	0/37/135/135	0/0/9/9
11	CLA	A	1110	-	-	0/23/122/135	0/0/9/9
11	CLA	A	1111	-	-	0/31/129/135	0/0/9/9
11	CLA	A	1112	-	-	0/11/111/135	0/0/9/9
11	CLA	A	1113	-	-	0/11/111/135	0/0/9/9
11	CLA	A	1114	-	-	0/15/113/135	0/0/9/9
11	CLA	A	1115	-	-	0/15/113/135	0/0/9/9
11	CLA	A	1116	-	-	0/23/122/135	0/0/9/9
11	CLA	A	1117	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1118	-	-	0/33/131/135	0/0/9/9
11	CLA	A	1119	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1120	-	-	0/15/113/135	0/0/9/9
11	CLA	A	1121	-	-	0/15/113/135	0/0/9/9
11	CLA	A	1122	-	-	0/29/128/135	0/0/9/9
11	CLA	A	1123	-	-	1/37/135/135	0/0/9/9
11	CLA	A	1124	-	-	0/25/123/135	0/0/9/9
11	CLA	A	1125	-	-	0/22/120/135	0/0/9/9
11	CLA	A	1126	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1127	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1128	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1129	-	-	0/15/113/135	0/0/9/9
11	CLA	A	1130	-	-	0/15/113/135	0/0/9/9
11	CLA	A	1131	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1132	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1133	-	-	0/15/113/135	0/0/9/9
11	CLA	A	1134	1	-	0/15/113/135	0/0/9/9
11	CLA	A	1135	-	-	0/21/119/135	0/0/9/9
11	CLA	A	1136	-	-	0/15/113/135	0/0/9/9
11	CLA	A	1137	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1138	-	-	0/15/113/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	1139	-	-	0/19/117/135	0/0/9/9
11	CLA	A	1140	-	-	0/37/135/135	0/0/9/9
11	CLA	A	1237	-	-	0/25/123/135	0/0/9/9
11	CLA	A	1801	15	-	0/22/120/135	0/0/9/9
12	PQN	A	2001	-	-	0/23/43/43	0/2/2/2
13	SF4	A	3001	1,2	-	0/0/48/48	0/6/5/5
14	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4008	-	-	3/29/63/63	0/2/2/2
15	LHG	A	5001	-	-	0/53/53/53	0/0/0/0
15	LHG	A	5003	11	-	0/53/53/53	0/0/0/0
11	CLA	B	1013	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1021	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1023	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1201	-	-	0/23/122/135	0/0/9/9
11	CLA	B	1202	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1203	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1204	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1205	-	-	0/25/123/135	0/0/9/9
11	CLA	B	1206	2	-	0/37/135/135	0/0/9/9
11	CLA	B	1207	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1208	-	-	0/11/111/135	0/0/9/9
11	CLA	B	1209	-	-	0/11/111/135	0/0/9/9
11	CLA	B	1210	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1211	-	-	0/15/113/135	0/0/9/9
11	CLA	B	1212	-	-	0/11/111/135	0/0/9/9
11	CLA	B	1213	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1214	-	-	0/29/128/135	0/0/9/9
11	CLA	B	1215	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1216	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1217	-	-	0/16/114/135	0/0/9/9
11	CLA	B	1218	-	-	0/11/111/135	0/0/9/9
11	CLA	B	1219	-	-	0/25/123/135	0/0/9/9
11	CLA	B	1220	-	-	0/15/113/135	0/0/9/9
11	CLA	B	1221	-	-	0/23/122/135	0/0/9/9
11	CLA	B	1222	-	-	0/27/125/135	0/0/9/9
11	CLA	B	1223	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1224	-	-	0/25/123/135	0/0/9/9
11	CLA	B	1225	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1226	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1227	-	-	0/11/111/135	0/0/9/9
11	CLA	B	1228	-	-	0/19/117/135	0/0/9/9
11	CLA	B	1229	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1230	-	-	1/29/127/135	0/0/9/9
11	CLA	B	1231	-	-	0/11/111/135	0/0/9/9
11	CLA	B	1232	-	-	0/11/111/135	0/0/9/9
11	CLA	B	1234	-	-	0/31/129/135	0/0/9/9
11	CLA	B	1235	-	-	0/31/129/135	0/0/9/9
11	CLA	B	1236	-	-	0/16/114/135	0/0/9/9
11	CLA	B	1238	-	-	0/37/135/135	0/0/9/9
11	CLA	B	1239	-	-	0/15/113/135	0/0/9/9
11	CLA	B	1240	15	-	0/11/111/135	0/0/9/9
12	PQN	B	2002	-	-	0/23/43/43	0/2/2/2
14	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4005	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4006	-	-	2/29/63/63	0/2/2/2
14	BCR	B	4009	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4010	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4011	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4014	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4017	-	-	1/29/63/63	0/2/2/2
16	LMG	B	5002	-	-	0/50/70/70	0/1/1/1
15	LHG	B	5004	11	-	0/53/53/53	0/0/0/0
13	SF4	C	3002	3	-	0/0/48/48	0/6/5/5
13	SF4	C	3003	3	-	0/0/48/48	0/6/5/5
14	BCR	F	4013	-	-	0/29/63/63	0/2/2/2
14	BCR	F	4018	-	-	0/29/63/63	0/2/2/2
14	BCR	F	4020	-	-	0/29/63/63	0/2/2/2
11	CLA	K	1401	-	-	0/37/135/135	0/0/9/9
11	CLA	K	1402	-	-	0/19/117/135	0/0/9/9
11	CLA	L	1501	7	-	0/37/135/135	0/0/9/9
11	CLA	L	1502	-	-	0/15/113/135	0/0/9/9
11	CLA	L	1503	-	-	1/37/135/135	0/0/9/9
14	BCR	L	4019	-	-	0/29/63/63	0/2/2/2
14	BCR	L	4022	-	-	0/29/63/63	0/2/2/2
14	BCR	M	4021	-	-	0/29/63/63	0/2/2/2
11	CLA	a	1011	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1012	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1022	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1101	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1102	11	-	0/37/135/135	0/0/9/9
11	CLA	a	1103	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	a	1104	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1105	-	-	0/17/115/135	0/0/9/9
11	CLA	a	1106	1	-	0/37/135/135	0/0/9/9
11	CLA	a	1107	1	-	0/37/135/135	0/0/9/9
11	CLA	a	1108	-	-	0/11/111/135	0/0/9/9
11	CLA	a	1109	11	-	0/37/135/135	0/0/9/9
11	CLA	a	1110	-	-	0/23/122/135	0/0/9/9
11	CLA	a	1111	-	-	0/31/129/135	0/0/9/9
11	CLA	a	1112	-	-	0/11/111/135	0/0/9/9
11	CLA	a	1113	-	-	0/11/111/135	0/0/9/9
11	CLA	a	1114	-	-	0/15/113/135	0/0/9/9
11	CLA	a	1115	-	-	0/15/113/135	0/0/9/9
11	CLA	a	1116	-	-	0/23/122/135	0/0/9/9
11	CLA	a	1117	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1118	-	-	0/33/131/135	0/0/9/9
11	CLA	a	1119	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1120	-	-	0/15/113/135	0/0/9/9
11	CLA	a	1121	-	-	0/15/113/135	0/0/9/9
11	CLA	a	1122	-	-	0/29/128/135	0/0/9/9
11	CLA	a	1123	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1124	-	-	0/25/123/135	0/0/9/9
11	CLA	a	1125	-	-	0/22/120/135	0/0/9/9
11	CLA	a	1126	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1127	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1128	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1129	-	-	0/15/113/135	0/0/9/9
11	CLA	a	1130	-	-	0/15/113/135	0/0/9/9
11	CLA	a	1131	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1132	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1133	-	-	0/15/113/135	0/0/9/9
11	CLA	a	1134	-	-	0/15/113/135	0/0/9/9
11	CLA	a	1135	-	-	0/21/119/135	0/0/9/9
11	CLA	a	1136	-	-	0/15/113/135	0/0/9/9
11	CLA	a	1137	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1138	-	-	0/15/113/135	0/0/9/9
11	CLA	a	1139	-	-	0/19/117/135	0/0/9/9
11	CLA	a	1140	-	-	0/37/135/135	0/0/9/9
11	CLA	a	1237	-	-	0/25/123/135	0/0/9/9
11	CLA	a	1801	15	-	0/22/120/135	0/0/9/9
12	PQN	a	2001	-	-	0/23/43/43	0/2/2/2
13	SF4	a	3001	1,2	-	0/0/48/48	0/6/5/5
14	BCR	a	4001	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	a	4002	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4003	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4007	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4008	-	-	1/29/63/63	0/2/2/2
15	LHG	a	5001	-	-	0/53/53/53	0/0/0/0
15	LHG	a	5003	11	-	0/53/53/53	0/0/0/0
11	CLA	b	1013	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1021	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1023	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1201	-	-	0/23/122/135	0/0/9/9
11	CLA	b	1202	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1203	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1204	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1205	-	-	0/25/123/135	0/0/9/9
11	CLA	b	1206	2	-	0/37/135/135	0/0/9/9
11	CLA	b	1207	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1208	-	-	0/11/111/135	0/0/9/9
11	CLA	b	1209	-	-	0/11/111/135	0/0/9/9
11	CLA	b	1210	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1211	-	-	0/15/113/135	0/0/9/9
11	CLA	b	1212	-	-	0/11/111/135	0/0/9/9
11	CLA	b	1213	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1214	-	-	0/29/128/135	0/0/9/9
11	CLA	b	1215	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1216	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1217	-	-	0/16/114/135	0/0/9/9
11	CLA	b	1218	-	-	0/11/111/135	0/0/9/9
11	CLA	b	1219	-	-	0/25/123/135	0/0/9/9
11	CLA	b	1220	-	-	0/15/113/135	0/0/9/9
11	CLA	b	1221	-	-	0/23/122/135	0/0/9/9
11	CLA	b	1222	-	-	0/27/125/135	0/0/9/9
11	CLA	b	1223	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1224	-	-	0/25/123/135	0/0/9/9
11	CLA	b	1225	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1226	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1227	-	-	0/11/111/135	0/0/9/9
11	CLA	b	1228	-	-	0/19/117/135	0/0/9/9
11	CLA	b	1229	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1230	-	-	0/29/127/135	0/0/9/9
11	CLA	b	1231	-	-	0/11/111/135	0/0/9/9
11	CLA	b	1232	-	-	0/11/111/135	0/0/9/9
11	CLA	b	1234	-	-	0/31/129/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1235	-	-	0/31/129/135	0/0/9/9
11	CLA	b	1236	-	-	0/16/114/135	0/0/9/9
11	CLA	b	1238	-	-	0/37/135/135	0/0/9/9
11	CLA	b	1239	-	-	0/15/113/135	0/0/9/9
11	CLA	b	1240	-	-	0/11/111/135	0/0/9/9
12	PQN	b	2002	-	-	0/23/43/43	0/2/2/2
14	BCR	b	4004	-	-	1/29/63/63	0/2/2/2
14	BCR	b	4005	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4006	-	-	2/29/63/63	0/2/2/2
14	BCR	b	4009	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4010	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4011	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4014	-	-	2/29/63/63	0/2/2/2
14	BCR	b	4017	-	-	1/29/63/63	0/2/2/2
16	LMG	b	5002	-	-	0/50/70/70	0/1/1/1
15	LHG	b	5004	-	-	0/53/53/53	0/0/0/0
13	SF4	c	3002	3	-	0/0/48/48	0/6/5/5
13	SF4	c	3003	3	-	0/0/48/48	0/6/5/5
14	BCR	f	4013	-	-	0/29/63/63	0/2/2/2
14	BCR	f	4018	-	-	0/29/63/63	0/2/2/2
14	BCR	f	4020	-	-	0/29/63/63	0/2/2/2
11	CLA	k	1401	-	-	0/37/135/135	0/0/9/9
11	CLA	k	1402	-	-	0/19/117/135	0/0/9/9
11	CLA	l	1501	7	-	0/37/135/135	0/0/9/9
11	CLA	l	1502	-	-	0/15/113/135	0/0/9/9
11	CLA	l	1503	-	-	0/37/135/135	0/0/9/9
14	BCR	l	4019	-	-	0/29/63/63	0/2/2/2
14	BCR	l	4022	-	-	0/29/63/63	0/2/2/2
14	BCR	m	4021	-	-	0/29/63/63	0/2/2/2

The worst 5 of 5992 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1217	CLA	O2A-C1	11.06	1.61	1.45
11	2	1217	CLA	O2A-C1	10.91	1.61	1.45
11	B	1236	CLA	O2A-C1	10.90	1.61	1.45
11	b	1236	CLA	O2A-C1	10.84	1.61	1.45
11	2	1236	CLA	O2A-C1	10.72	1.60	1.45

The worst 5 of 8442 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4002	BCR	C16-C17-C18	28.20	168.05	127.29
14	b	4009	BCR	C16-C17-C18	27.52	167.07	127.29
14	6	4013	BCR	C20-C21-C22	25.70	164.43	127.29
14	F	4013	BCR	C20-C21-C22	25.42	164.03	127.29
14	f	4013	BCR	C20-C21-C22	25.06	163.51	127.29

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1123	CLA	CGA-O2A-C1-C2
11	A	1022	CLA	CGA-O2A-C1-C2
11	B	1230	CLA	CGA-O2A-C1-C2
11	1	1119	CLA	CGA-O2A-C1-C2
11	L	1503	CLA	CGA-O2A-C1-C2

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 failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.