Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:07 PM GMT

PDB ID	:	1ILX
Title	:	Excited State Dynamics in Photosystem II Revised. New Insights from the X-ray Structure.
Authors	:	Vasilev, S.; Orth, P.; Zouni, A.; Owens, T.G.; Bruce, D.
Deposited on	:	2001-05-09
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

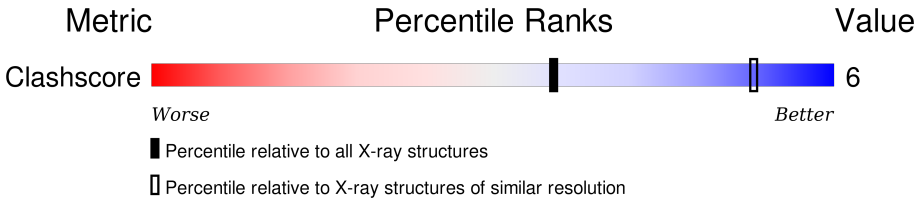
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	102246	1458 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	169	97% .
1	J	169	97% .
2	B	174	97% .
2	K	174	97% .
3	C	156	99% .
3	L	156	99% .
4	D	155	99% .
4	M	155	99% .
5	E	40	100%

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Mol	Chain	Length	Quality of chain
5	N	40	100%
6	F	30	100%
6	O	30	100%
7	G	312	100%
7	P	312	100%
8	H	115	100%
8	Q	115	100%
9	I	87	100%
9	R	87	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	174	X	-	-	-
13	CLA	A	175	X	-	-	-
13	CLA	A	176	X	-	-	-
13	CLA	A	178	X	-	-	-
13	CLA	A	179	X	-	-	-
13	CLA	B	176	X	-	-	-
13	CLA	B	178	X	-	-	-
13	CLA	C	157	X	-	-	-
13	CLA	C	158	X	-	-	-
13	CLA	C	159	X	-	-	-
13	CLA	C	160	X	-	-	-
13	CLA	C	161	X	-	-	-
13	CLA	C	162	X	-	-	-
13	CLA	C	163	X	-	-	-
13	CLA	C	164	X	-	-	-
13	CLA	C	165	X	-	-	-
13	CLA	C	166	X	-	-	-
13	CLA	C	167	X	-	-	-
13	CLA	C	168	X	-	-	-
13	CLA	D	156	X	-	-	-
13	CLA	D	157	X	-	-	-
13	CLA	D	158	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	D	159	X	-	-	-
13	CLA	D	160	X	-	-	-
13	CLA	D	161	X	-	-	-
13	CLA	D	162	X	-	-	-
13	CLA	D	163	X	-	-	-
13	CLA	D	164	X	-	-	-
13	CLA	D	165	X	-	-	-
13	CLA	D	166	X	-	-	-
13	CLA	D	167	X	-	-	-
13	CLA	D	168	X	-	-	-
13	CLA	D	169	X	-	-	-
13	CLA	D	170	X	-	-	-
13	CLA	G	313	X	-	-	-
13	CLA	J	174	X	-	-	-
13	CLA	J	175	X	-	-	-
13	CLA	J	176	X	-	-	-
13	CLA	J	178	X	-	-	-
13	CLA	J	179	X	-	-	-
13	CLA	K	176	X	-	-	-
13	CLA	K	178	X	-	-	-
13	CLA	L	157	X	-	-	-
13	CLA	L	158	X	-	-	-
13	CLA	L	159	X	-	-	-
13	CLA	L	160	X	-	-	-
13	CLA	L	161	X	-	-	-
13	CLA	L	162	X	-	-	-
13	CLA	L	163	X	-	-	-
13	CLA	L	164	X	-	-	-
13	CLA	L	165	X	-	-	-
13	CLA	L	166	X	-	-	-
13	CLA	L	167	X	-	-	-
13	CLA	L	168	X	-	-	-
13	CLA	M	156	X	-	-	-
13	CLA	M	157	X	-	-	-
13	CLA	M	158	X	-	-	-
13	CLA	M	159	X	-	-	-
13	CLA	M	160	X	-	-	-
13	CLA	M	161	X	-	-	-
13	CLA	M	162	X	-	-	-
13	CLA	M	163	X	-	-	-
13	CLA	M	164	X	-	-	-
13	CLA	M	165	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	M	166	X	-	-	-
13	CLA	M	167	X	-	-	-
13	CLA	M	168	X	-	-	-
13	CLA	M	169	X	-	-	-
13	CLA	M	170	X	-	-	-
13	CLA	P	313	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 4594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 II: SUBUNIT PSBA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	169	Total C 169 169	0	0	169
1	J	169	Total C 169 169	0	0	169

- Molecule 2 is a protein called PHOTOSYSTEM II: SUBUNIT PSBD.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	174	Total C 174 174	0	0	174
2	K	174	Total C 174 174	0	0	174

- Molecule 3 is a protein called PHOTOSYSTEM II: SUBUNIT PSBC.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	156	Total C 156 156	0	0	156
3	L	156	Total C 156 156	0	0	156

- Molecule 4 is a protein called PHOTOSYSTEM II: SUBUNIT PSBB.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	155	Total C 155 155	0	0	155
4	M	155	Total C 155 155	0	0	155

- Molecule 5 is a protein called PHOTOSYSTEM II: SUBUNIT PSBE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	40	Total C 40 40	0	0	40
5	N	40	Total C 40 40	0	0	40

- Molecule 6 is a protein called PHOTOSYSTEM II: SUBUNIT PSBF.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	30	Total C 30 30	0	0	30
6	O	30	Total C 30 30	0	0	30

- Molecule 7 is a protein called PHOTOSYSTEM II: SUBUNIT UNKNOWN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	312	Total C 312 312	0	0	312
7	P	312	Total C 312 312	0	0	312

- Molecule 8 is a protein called PHOTOSYSTEM II: SUBUNIT PSBO.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	115	Total C 115 115	0	0	115
8	Q	115	Total C 115 115	0	0	115

- Molecule 9 is a protein called PHOTOSYSTEM II: SUBUNIT PSBV.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	87	Total C 87 87	0	0	87
9	R	87	Total C 87 87	0	0	87

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	J	4	Total Mn 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	4	Total Mn 4 4	0	0

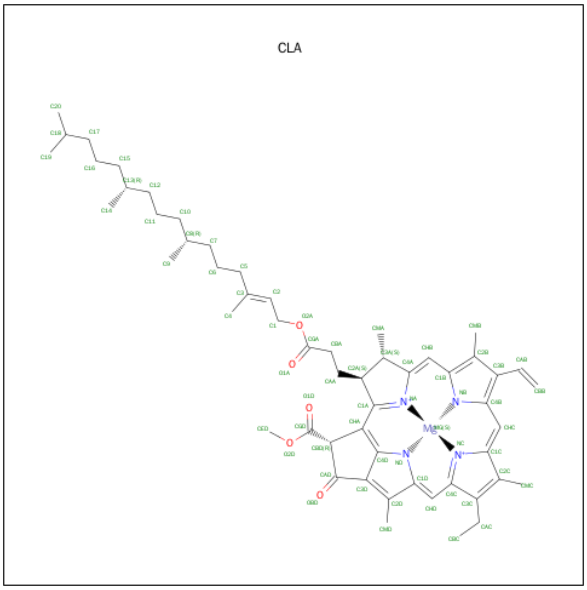
- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Fe 1 1	0	0
11	K	1	Total Fe 1 1	0	0

- Molecule 12 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	H	1	Total Cd 1 1	0	0
12	Q	1	Total Cd 1 1	0	0

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C Mg N 27 22 1 4	0	0
13	B	1	Total C Mg N 27 22 1 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C Mg N 27 22 1 4	0	0
13	A	1	Total C Mg N 27 22 1 4	0	0
13	A	1	Total C Mg N 27 22 1 4	0	0
13	B	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	A	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	C	1	Total C Mg N 27 22 1 4	0	0
13	G	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	D	1	Total C Mg N 27 22 1 4	0	0
13	J	1	Total C Mg N 27 22 1 4	0	0
13	K	1	Total C Mg N 27 22 1 4	0	0
13	J	1	Total C Mg N 27 22 1 4	0	0
13	J	1	Total C Mg N 27 22 1 4	0	0
13	J	1	Total C Mg N 27 22 1 4	0	0
13	K	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	J	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	L	1	Total C Mg N 27 22 1 4	0	0
13	P	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0

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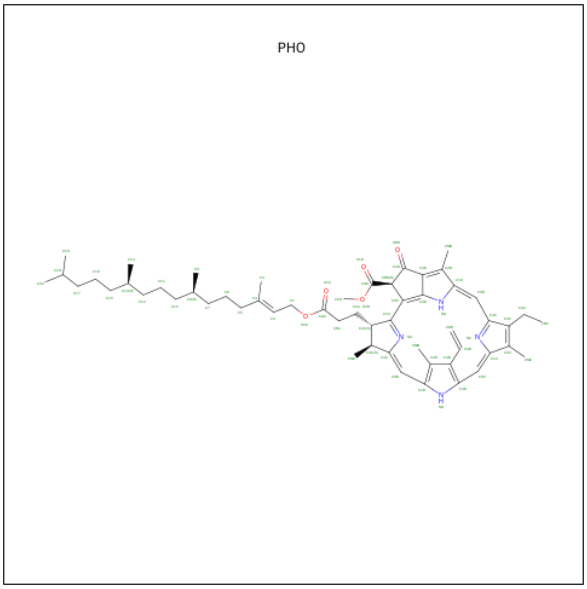
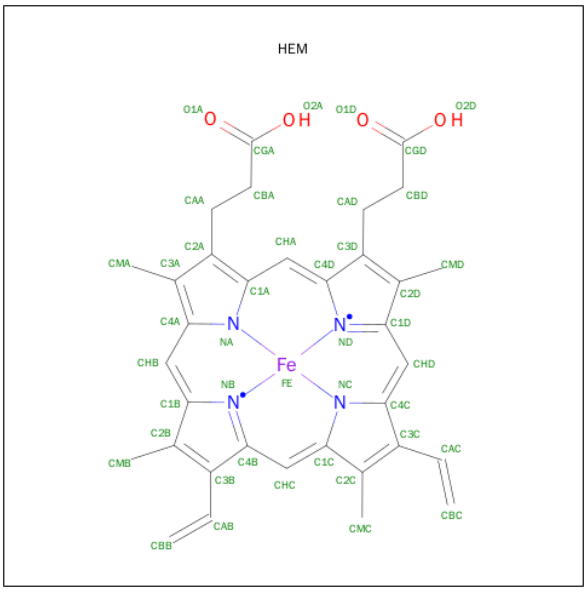
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0
13	M	1	Total C Mg N 27 22 1 4	0	0

- Molecule 14 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



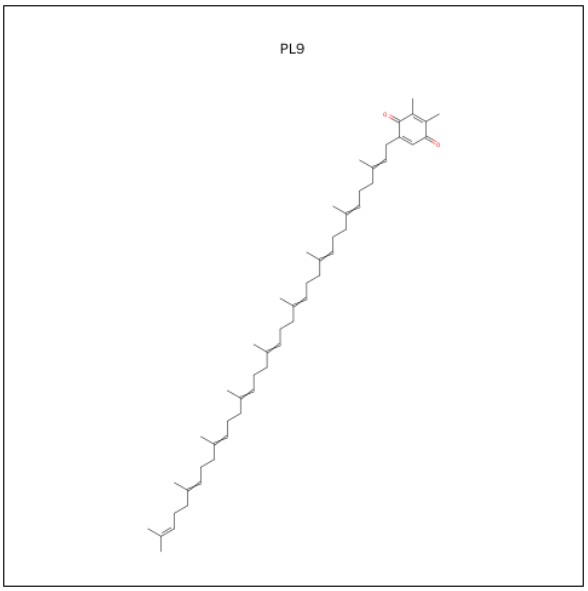
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C N 26 22 4	0	0
14	A	1	Total C N 26 22 4	0	0
14	K	1	Total C N 26 22 4	0	0
14	J	1	Total C N 26 22 4	0	0

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	F	1	Total	C	Fe	N	0	0
			25	20	1	4		
15	I	1	Total	C	Fe	N	0	0
			25	20	1	4		
15	O	1	Total	C	Fe	N	0	0
			25	20	1	4		
15	R	1	Total	C	Fe	N	0	0
			25	20	1	4		

- Molecule 16 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C 6 6	0	0
16	K	1	Total C 6 6	0	0

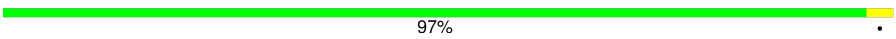
3 Residue-property plots (i)

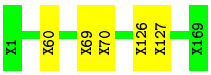
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

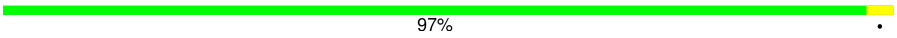
Chain A:

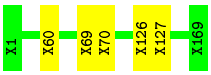




- Molecule 1: PHOTOSYSTEM II: SUBUNIT PSBA

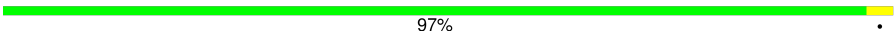
Chain J:

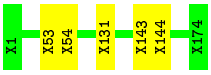




- Molecule 2: PHOTOSYSTEM II: SUBUNIT PSBD

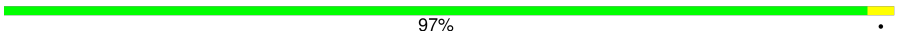
Chain B:

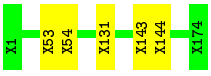




- Molecule 2: PHOTOSYSTEM II: SUBUNIT PSBD

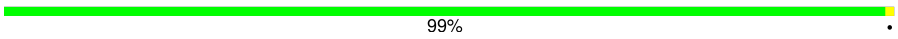
Chain K:

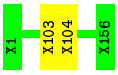




- Molecule 3: PHOTOSYSTEM II: SUBUNIT PSBC

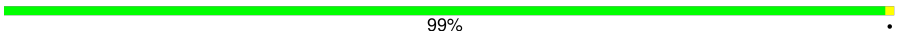
Chain C:

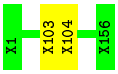




- Molecule 3: PHOTOSYSTEM II: SUBUNIT PSBC

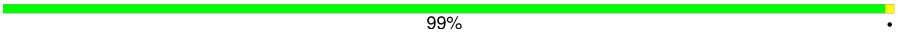
Chain L:





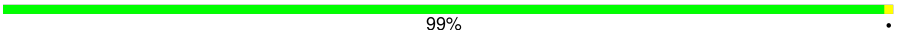
• Molecule 4: PHOTOSYSTEM II: SUBUNIT PSBB

Chain D:



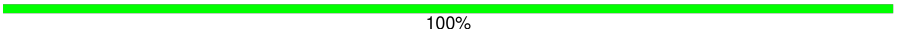
• Molecule 4: PHOTOSYSTEM II: SUBUNIT PSBB

Chain M:



• Molecule 5: PHOTOSYSTEM II: SUBUNIT PSBE

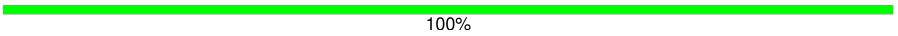
Chain E:



There are no outlier residues recorded for this chain.

• Molecule 5: PHOTOSYSTEM II: SUBUNIT PSBE

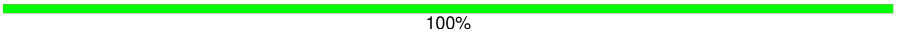
Chain N:



There are no outlier residues recorded for this chain.

• Molecule 6: PHOTOSYSTEM II: SUBUNIT PSBF

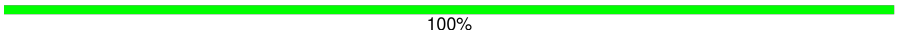
Chain F:



There are no outlier residues recorded for this chain.

• Molecule 6: PHOTOSYSTEM II: SUBUNIT PSBF

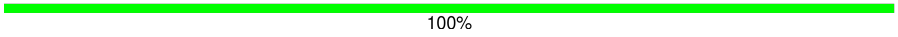
Chain O:



There are no outlier residues recorded for this chain.

• Molecule 7: PHOTOSYSTEM II: SUBUNIT UNKNOWN

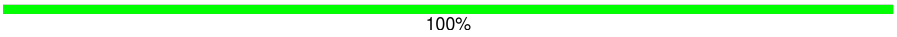
Chain G:



There are no outlier residues recorded for this chain.

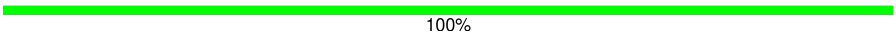
• Molecule 7: PHOTOSYSTEM II: SUBUNIT UNKNOWN

Chain P:



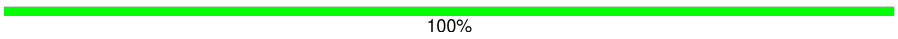
There are no outlier residues recorded for this chain.

• Molecule 8: PHOTOSYSTEM II: SUBUNIT PSBO

Chain H: 

There are no outlier residues recorded for this chain.

- Molecule 8: PHOTOSYSTEM II: SUBUNIT PSBO

Chain Q: 

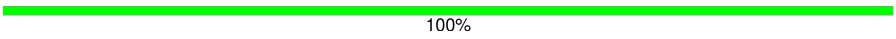
There are no outlier residues recorded for this chain.

- Molecule 9: PHOTOSYSTEM II: SUBUNIT PSBV

Chain I: 

There are no outlier residues recorded for this chain.

- Molecule 9: PHOTOSYSTEM II: SUBUNIT PSBV

Chain R: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	130.01Å 226.72Å 308.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	?	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4594	wwPDB-VP
Average B, all atoms (Å^2)	1.0	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: PHO, MN, CLA, PL9, CD, FE, HEM

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 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	169	0	0	4	0
1	J	169	0	0	4	0
2	B	174	0	0	4	0
2	K	174	0	0	4	0
3	C	156	0	0	2	0
3	L	156	0	0	2	0
4	D	155	0	0	3	0
4	M	155	0	0	3	0
5	E	40	0	0	0	0
5	N	40	0	0	0	0
6	F	30	0	0	0	0
6	O	30	0	0	0	0
7	G	312	0	0	0	0
7	P	312	0	0	0	0
8	H	115	0	0	0	0
8	Q	115	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	87	0	0	0	0
9	R	87	0	0	0	0
10	A	4	0	0	0	0
10	J	4	0	0	0	0
11	B	1	0	0	0	0
11	K	1	0	0	0	0
12	H	1	0	0	0	0
12	Q	1	0	0	0	0
13	A	135	0	15	0	0
13	B	54	0	6	0	0
13	C	324	0	36	2	0
13	D	405	0	45	7	0
13	G	27	0	3	4	0
13	J	135	0	15	0	0
13	K	54	0	6	0	0
13	L	324	0	36	2	0
13	M	405	0	45	7	0
13	P	27	0	3	4	0
14	A	26	0	5	0	0
14	B	26	0	5	0	0
14	J	26	0	5	0	0
14	K	26	0	5	0	0
15	F	25	0	4	0	0
15	I	25	0	4	0	0
15	O	25	0	4	0	0
15	R	25	0	4	0	0
16	B	6	0	1	0	0
16	K	6	0	1	0	0
All	All	4594	0	248	28	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:UNK:CA	2:K:53:UNK:CA	1.88	1.51
1:A:127:UNK:CA	2:B:53:UNK:CA	1.88	1.49
1:A:60:UNK:CA	2:B:131:UNK:CA	1.95	1.45
1:J:60:UNK:CA	2:K:131:UNK:CA	1.95	1.44
3:L:103:UNK:CA	13:L:168:CLA:C2A	2.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:UNK:CA	13:C:168:CLA:C2A	2.41	0.98
13:M:168:CLA:CAD	13:P:313:CLA:CAD	2.54	0.85
13:D:168:CLA:CAD	13:G:313:CLA:CAD	2.54	0.85
1:J:126:UNK:CA	2:K:54:UNK:CA	2.66	0.74
1:A:126:UNK:CA	2:B:54:UNK:CA	2.66	0.73
13:M:168:CLA:CBD	13:P:313:CLA:CAD	2.68	0.72
13:D:168:CLA:CBD	13:G:313:CLA:CAD	2.68	0.70
1:A:69:UNK:CA	1:A:70:UNK:CA	2.76	0.64
1:J:69:UNK:CA	1:J:70:UNK:CA	2.76	0.63
4:D:22:UNK:CA	13:D:165:CLA:CHC	2.77	0.62
4:M:22:UNK:CA	13:M:165:CLA:CHC	2.77	0.62
4:D:22:UNK:CA	13:D:165:CLA:C4B	2.80	0.60
4:M:22:UNK:CA	13:M:165:CLA:C3B	2.81	0.59
4:M:22:UNK:CA	13:M:165:CLA:C4B	2.80	0.59
4:D:22:UNK:CA	13:D:165:CLA:C3B	2.81	0.58
13:M:168:CLA:CHA	13:P:313:CLA:CBD	2.90	0.50
13:D:168:CLA:CHA	13:G:313:CLA:CBD	2.90	0.49
2:B:143:UNK:CA	2:B:144:UNK:CA	2.91	0.48
2:K:143:UNK:CA	2:K:144:UNK:CA	2.91	0.48
3:L:104:UNK:CA	13:L:168:CLA:CBD	2.94	0.45
3:C:104:UNK:CA	13:C:168:CLA:CBD	2.94	0.45
13:D:168:CLA:C3D	13:G:313:CLA:CAD	2.98	0.41
13:M:168:CLA:C3D	13:P:313:CLA:CAD	2.98	0.41

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 molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 92 ligands modelled in this entry, 12 are monoatomic - leaving 80 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	$\#\|Z\| > 2$
13	CLA	A	174	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	A	175	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	A	176	-	18,35,73	2.37	4 (22%)	22,60,113	1.74	4 (18%)
14	PHO	A	177	-	28,31,69	1.43	4 (14%)	30,46,99	1.17	2 (6%)
13	CLA	A	178	-	18,35,73	2.38	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	A	179	-	18,35,73	2.39	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	B	176	-	18,35,73	2.37	4 (22%)	22,60,113	1.73	4 (18%)
14	PHO	B	177	-	28,31,69	1.42	4 (14%)	30,46,99	1.17	2 (6%)
13	CLA	B	178	-	18,35,73	2.39	4 (22%)	22,60,113	1.73	4 (18%)
16	PL9	B	179	-	6,6,55	2.74	2 (33%)	6,6,69	0.83	0
13	CLA	C	157	-	18,35,73	2.38	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	C	158	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	C	159	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	C	160	-	18,35,73	2.37	4 (22%)	22,60,113	1.72	4 (18%)
13	CLA	C	161	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	C	162	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	C	163	-	18,35,73	2.38	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	C	164	-	18,35,73	2.39	4 (22%)	22,60,113	1.73	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	C	165	-	18,35,73	2.39	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	C	166	-	18,35,73	2.39	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	C	167	-	18,35,73	2.41	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	C	168	-	18,35,73	2.39	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	D	156	-	18,35,73	2.39	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	D	157	-	18,35,73	2.37	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	D	158	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	D	159	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	D	160	-	18,35,73	2.40	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	D	161	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	D	162	-	18,35,73	2.39	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	D	163	-	18,35,73	2.40	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	D	164	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	D	165	-	18,35,73	2.39	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	D	166	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	D	167	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	D	168	-	18,35,73	2.38	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	D	169	-	18,35,73	2.37	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	D	170	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
15	HEM	F	50	-	25,32,50	3.92	11 (44%)	22,54,82	2.94	10 (45%)
13	CLA	G	313	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
15	HEM	I	88	-	25,32,50	3.94	11 (44%)	22,54,82	2.98	10 (45%)
13	CLA	J	174	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	J	175	-	18,35,73	2.40	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	J	176	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
14	PHO	J	177	-	28,31,69	1.43	4 (14%)	30,46,99	1.18	2 (6%)
13	CLA	J	178	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	J	179	-	18,35,73	2.40	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	K	176	-	18,35,73	2.37	4 (22%)	22,60,113	1.72	4 (18%)
14	PHO	K	177	-	28,31,69	1.42	4 (14%)	30,46,99	1.16	2 (6%)
13	CLA	K	178	-	18,35,73	2.39	4 (22%)	22,60,113	1.72	4 (18%)
16	PL9	K	179	-	6,6,55	2.74	2 (33%)	6,6,69	0.83	0
13	CLA	L	157	-	18,35,73	2.38	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	L	158	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	L	159	-	18,35,73	2.39	4 (22%)	22,60,113	1.73	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	L	160	-	18,35,73	2.37	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	L	161	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	L	162	-	18,35,73	2.38	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	L	163	-	18,35,73	2.37	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	L	164	-	18,35,73	2.39	4 (22%)	22,60,113	1.72	4 (18%)
13	CLA	L	165	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	L	166	-	18,35,73	2.39	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	L	167	-	18,35,73	2.41	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	L	168	-	18,35,73	2.40	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	M	156	-	18,35,73	2.40	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	M	157	-	18,35,73	2.37	4 (22%)	22,60,113	1.72	4 (18%)
13	CLA	M	158	-	18,35,73	2.39	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	M	159	-	18,35,73	2.40	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	M	160	-	18,35,73	2.40	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	M	161	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	M	162	-	18,35,73	2.39	5 (27%)	22,60,113	1.73	4 (18%)
13	CLA	M	163	-	18,35,73	2.40	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	M	164	-	18,35,73	2.39	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	M	165	-	18,35,73	2.39	4 (22%)	22,60,113	1.74	4 (18%)
13	CLA	M	166	-	18,35,73	2.39	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	M	167	-	18,35,73	2.37	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	M	168	-	18,35,73	2.39	4 (22%)	22,60,113	1.75	4 (18%)
13	CLA	M	169	-	18,35,73	2.37	4 (22%)	22,60,113	1.73	4 (18%)
13	CLA	M	170	-	18,35,73	2.38	4 (22%)	22,60,113	1.73	4 (18%)
15	HEM	O	90	-	25,32,50	3.93	11 (44%)	22,54,82	2.92	10 (45%)
13	CLA	P	313	-	18,35,73	2.38	4 (22%)	22,60,113	1.74	4 (18%)
15	HEM	R	91	-	25,32,50	3.94	11 (44%)	22,54,82	2.98	10 (45%)

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
13	CLA	A	174	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	A	175	-	3/3/8/25	0/0/75/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	176	-	3/3/8/25	0/0/75/135	0/0/9/9
14	PHO	A	177	-	-	0/14/43/103	0/1/6/6
13	CLA	A	178	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	A	179	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	B	176	-	3/3/8/25	0/0/75/135	0/0/9/9
14	PHO	B	177	-	-	0/14/43/103	0/1/6/6
13	CLA	B	178	-	3/3/8/25	0/0/75/135	0/0/9/9
16	PL9	B	179	-	-	0/0/6/73	0/1/1/1
13	CLA	C	157	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	158	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	159	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	160	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	161	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	162	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	163	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	164	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	165	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	166	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	167	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	C	168	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	156	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	157	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	158	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	159	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	160	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	161	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	162	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	163	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	164	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	165	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	166	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	167	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	168	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	169	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	D	170	-	3/3/8/25	0/0/75/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEM	F	50	-	-	0/0/40/54	0/0/8/8
13	CLA	G	313	-	3/3/8/25	0/0/75/135	0/0/9/9
15	HEM	I	88	-	-	0/0/40/54	0/0/8/8
13	CLA	J	174	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	J	175	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	J	176	-	3/3/8/25	0/0/75/135	0/0/9/9
14	PHO	J	177	-	-	0/14/43/103	0/1/6/6
13	CLA	J	178	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	J	179	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	K	176	-	3/3/8/25	0/0/75/135	0/0/9/9
14	PHO	K	177	-	-	0/14/43/103	0/1/6/6
13	CLA	K	178	-	3/3/8/25	0/0/75/135	0/0/9/9
16	PL9	K	179	-	-	0/0/6/73	0/1/1/1
13	CLA	L	157	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	158	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	159	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	160	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	161	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	162	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	163	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	164	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	165	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	166	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	167	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	L	168	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	156	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	157	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	158	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	159	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	160	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	161	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	162	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	163	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	164	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	165	-	3/3/8/25	0/0/75/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	M	166	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	167	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	168	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	169	-	3/3/8/25	0/0/75/135	0/0/9/9
13	CLA	M	170	-	3/3/8/25	0/0/75/135	0/0/9/9
15	HEM	O	90	-	-	0/0/40/54	0/0/8/8
13	CLA	P	313	-	3/3/8/25	0/0/75/135	0/0/9/9
15	HEM	R	91	-	-	0/0/40/54	0/0/8/8

All (345) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	88	HEM	C2D-C1D	-8.40	1.38	1.50
15	R	91	HEM	C2D-C1D	-8.39	1.38	1.50
15	F	50	HEM	C2D-C1D	-8.32	1.38	1.50
15	O	90	HEM	C2D-C1D	-8.28	1.38	1.50
15	R	91	HEM	C2B-C1B	-7.49	1.39	1.50
15	I	88	HEM	C2B-C1B	-7.46	1.39	1.50
15	O	90	HEM	C2B-C1B	-7.39	1.39	1.50
15	F	50	HEM	C2B-C1B	-7.39	1.39	1.50
15	O	90	HEM	C3D-C4D	-6.77	1.40	1.50
15	F	50	HEM	C3D-C4D	-6.77	1.40	1.50
15	R	91	HEM	C3D-C4D	-6.76	1.40	1.50
15	I	88	HEM	C3D-C4D	-6.75	1.40	1.50
15	R	91	HEM	C3B-C4B	-6.31	1.41	1.50
15	I	88	HEM	C3B-C4B	-6.31	1.41	1.50
15	O	90	HEM	C3B-C4B	-6.31	1.41	1.50
15	F	50	HEM	C3B-C4B	-6.30	1.41	1.50
13	J	179	CLA	CAD-C3D	-5.69	1.42	1.51
13	A	174	CLA	CAD-C3D	-5.63	1.42	1.51
13	L	157	CLA	CAD-C3D	-5.63	1.42	1.51
13	C	167	CLA	CAD-C3D	-5.63	1.42	1.51
13	A	179	CLA	CAD-C3D	-5.62	1.42	1.51
13	C	168	CLA	CAD-C3D	-5.60	1.42	1.51
13	J	174	CLA	CAD-C3D	-5.60	1.42	1.51
13	L	167	CLA	CAD-C3D	-5.60	1.42	1.51
13	J	178	CLA	CAD-C3D	-5.60	1.42	1.51
13	M	163	CLA	CAD-C3D	-5.60	1.42	1.51
13	D	170	CLA	CAD-C3D	-5.60	1.42	1.51
13	L	168	CLA	CAD-C3D	-5.59	1.42	1.51
13	G	313	CLA	CAD-C3D	-5.59	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	178	CLA	CAD-C3D	-5.59	1.42	1.51
13	M	170	CLA	CAD-C3D	-5.59	1.42	1.51
13	C	157	CLA	CAD-C3D	-5.58	1.42	1.51
13	M	162	CLA	CAD-C3D	-5.58	1.42	1.51
13	C	165	CLA	CAD-C3D	-5.58	1.42	1.51
13	D	159	CLA	CAD-C3D	-5.58	1.42	1.51
13	M	165	CLA	CAD-C3D	-5.58	1.42	1.51
13	M	159	CLA	CAD-C3D	-5.58	1.42	1.51
13	D	167	CLA	CAD-C3D	-5.58	1.42	1.51
13	P	313	CLA	CAD-C3D	-5.58	1.42	1.51
13	A	178	CLA	CAD-C3D	-5.58	1.42	1.51
13	D	165	CLA	CAD-C3D	-5.58	1.42	1.51
13	L	166	CLA	CAD-C3D	-5.57	1.42	1.51
13	M	167	CLA	CAD-C3D	-5.57	1.42	1.51
13	L	160	CLA	CAD-C3D	-5.57	1.42	1.51
13	D	163	CLA	CAD-C3D	-5.57	1.42	1.51
13	J	175	CLA	CAD-C3D	-5.57	1.42	1.51
13	M	166	CLA	CAD-C3D	-5.57	1.42	1.51
13	L	165	CLA	CAD-C3D	-5.56	1.42	1.51
13	D	168	CLA	CAD-C3D	-5.56	1.42	1.51
13	C	158	CLA	CAD-C3D	-5.56	1.42	1.51
13	M	158	CLA	CAD-C3D	-5.56	1.42	1.51
13	D	166	CLA	CAD-C3D	-5.56	1.42	1.51
13	K	178	CLA	CAD-C3D	-5.56	1.42	1.51
13	D	158	CLA	CAD-C3D	-5.56	1.42	1.51
13	J	176	CLA	CAD-C3D	-5.56	1.42	1.51
13	M	156	CLA	CAD-C3D	-5.56	1.42	1.51
13	D	156	CLA	CAD-C3D	-5.55	1.42	1.51
13	M	168	CLA	CAD-C3D	-5.55	1.42	1.51
13	A	175	CLA	CAD-C3D	-5.54	1.42	1.51
13	C	164	CLA	CAD-C3D	-5.54	1.42	1.51
13	C	160	CLA	CAD-C3D	-5.54	1.42	1.51
13	L	158	CLA	CAD-C3D	-5.54	1.42	1.51
13	L	159	CLA	CAD-C3D	-5.54	1.42	1.51
13	C	161	CLA	CAD-C3D	-5.54	1.42	1.51
13	D	161	CLA	CAD-C3D	-5.54	1.42	1.51
13	D	162	CLA	CAD-C3D	-5.53	1.42	1.51
13	D	160	CLA	CAD-C3D	-5.53	1.42	1.51
13	D	169	CLA	CAD-C3D	-5.53	1.42	1.51
13	M	161	CLA	CAD-C3D	-5.53	1.42	1.51
13	C	166	CLA	CAD-C3D	-5.53	1.42	1.51
13	M	160	CLA	CAD-C3D	-5.52	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	159	CLA	CAD-C3D	-5.52	1.42	1.51
13	A	176	CLA	CAD-C3D	-5.52	1.42	1.51
13	L	164	CLA	CAD-C3D	-5.52	1.42	1.51
13	C	162	CLA	CAD-C3D	-5.52	1.42	1.51
13	L	161	CLA	CAD-C3D	-5.52	1.42	1.51
13	B	176	CLA	CAD-C3D	-5.51	1.42	1.51
13	C	163	CLA	CAD-C3D	-5.51	1.42	1.51
13	M	169	CLA	CAD-C3D	-5.49	1.42	1.51
13	D	164	CLA	CAD-C3D	-5.49	1.42	1.51
13	L	162	CLA	CAD-C3D	-5.49	1.42	1.51
13	L	163	CLA	CAD-C3D	-5.49	1.42	1.51
13	M	164	CLA	CAD-C3D	-5.49	1.42	1.51
13	K	176	CLA	CAD-C3D	-5.48	1.42	1.51
13	M	157	CLA	CAD-C3D	-5.45	1.42	1.51
13	D	157	CLA	CAD-C3D	-5.45	1.42	1.51
13	L	167	CLA	C1B-CHB	-4.28	1.34	1.43
13	M	168	CLA	C1B-CHB	-4.26	1.34	1.43
13	M	160	CLA	C1B-CHB	-4.25	1.34	1.43
13	L	164	CLA	C1B-CHB	-4.25	1.34	1.43
13	M	159	CLA	C1B-CHB	-4.25	1.34	1.43
13	C	167	CLA	C1B-CHB	-4.25	1.34	1.43
13	D	162	CLA	C1B-CHB	-4.24	1.34	1.43
13	D	160	CLA	C1B-CHB	-4.24	1.34	1.43
13	C	164	CLA	C1B-CHB	-4.24	1.34	1.43
13	D	165	CLA	C1B-CHB	-4.23	1.34	1.43
13	M	163	CLA	C1B-CHB	-4.23	1.34	1.43
13	C	163	CLA	C1B-CHB	-4.23	1.34	1.43
13	D	157	CLA	C1B-CHB	-4.23	1.34	1.43
13	D	159	CLA	C1B-CHB	-4.23	1.34	1.43
13	G	313	CLA	C1B-CHB	-4.23	1.34	1.43
13	M	166	CLA	C1B-CHB	-4.23	1.34	1.43
13	M	164	CLA	C1B-CHB	-4.23	1.34	1.43
13	M	162	CLA	C1B-CHB	-4.22	1.34	1.43
13	D	168	CLA	C1B-CHB	-4.22	1.34	1.43
13	C	162	CLA	C1B-CHB	-4.22	1.34	1.43
13	C	159	CLA	C1B-CHB	-4.22	1.34	1.43
13	D	156	CLA	C1B-CHB	-4.22	1.34	1.43
13	J	178	CLA	C1B-CHB	-4.22	1.34	1.43
13	J	176	CLA	C1B-CHB	-4.22	1.34	1.43
13	D	163	CLA	C1B-CHB	-4.21	1.34	1.43
13	M	161	CLA	C1B-CHB	-4.21	1.34	1.43
13	M	157	CLA	C1B-CHB	-4.21	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	178	CLA	C1B-CHB	-4.21	1.34	1.43
13	M	165	CLA	C1B-CHB	-4.21	1.34	1.43
15	R	91	HEM	C3D-C2D	-4.21	1.41	1.52
13	L	162	CLA	C1B-CHB	-4.21	1.34	1.43
15	O	90	HEM	C3D-C2D	-4.21	1.41	1.52
15	F	50	HEM	C3D-C2D	-4.21	1.41	1.52
13	C	168	CLA	C1B-CHB	-4.21	1.34	1.43
13	D	166	CLA	C1B-CHB	-4.21	1.34	1.43
13	J	175	CLA	C1B-CHB	-4.21	1.34	1.43
13	L	166	CLA	C1B-CHB	-4.20	1.34	1.43
13	A	176	CLA	C1B-CHB	-4.20	1.34	1.43
13	M	156	CLA	C1B-CHB	-4.20	1.34	1.43
13	K	176	CLA	C1B-CHB	-4.20	1.34	1.43
13	L	161	CLA	C1B-CHB	-4.20	1.34	1.43
13	D	164	CLA	C1B-CHB	-4.20	1.34	1.43
13	L	163	CLA	C1B-CHB	-4.20	1.34	1.43
13	K	178	CLA	C1B-CHB	-4.20	1.34	1.43
13	D	158	CLA	C1B-CHB	-4.20	1.34	1.43
13	L	168	CLA	C1B-CHB	-4.20	1.34	1.43
13	A	175	CLA	C1B-CHB	-4.20	1.34	1.43
13	C	165	CLA	C1B-CHB	-4.20	1.34	1.43
15	I	88	HEM	C3D-C2D	-4.19	1.41	1.52
13	D	161	CLA	C1B-CHB	-4.19	1.34	1.43
13	L	159	CLA	C1B-CHB	-4.19	1.34	1.43
13	B	178	CLA	C1B-CHB	-4.19	1.34	1.43
13	D	169	CLA	C1B-CHB	-4.19	1.34	1.43
13	P	313	CLA	C1B-CHB	-4.19	1.34	1.43
13	C	166	CLA	C1B-CHB	-4.19	1.34	1.43
14	K	177	PHO	CAD-C3D	-4.19	1.42	1.50
13	D	170	CLA	C1B-CHB	-4.19	1.34	1.43
13	B	176	CLA	C1B-CHB	-4.19	1.34	1.43
14	J	177	PHO	CAD-C3D	-4.19	1.42	1.50
14	A	177	PHO	CAD-C3D	-4.19	1.42	1.50
13	A	174	CLA	C1B-CHB	-4.18	1.34	1.43
13	L	165	CLA	C1B-CHB	-4.18	1.34	1.43
13	D	167	CLA	C1B-CHB	-4.18	1.34	1.43
13	M	158	CLA	C1B-CHB	-4.18	1.34	1.43
14	B	177	PHO	CAD-C3D	-4.18	1.42	1.50
13	M	169	CLA	C1B-CHB	-4.18	1.34	1.43
13	C	160	CLA	C1B-CHB	-4.18	1.34	1.43
13	L	160	CLA	C1B-CHB	-4.17	1.34	1.43
13	C	161	CLA	C1B-CHB	-4.17	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	167	CLA	C1B-CHB	-4.17	1.34	1.43
13	C	158	CLA	C1B-CHB	-4.17	1.34	1.43
13	C	157	CLA	C1B-CHB	-4.17	1.35	1.43
13	J	174	CLA	C1B-CHB	-4.16	1.35	1.43
13	A	179	CLA	C1B-CHB	-4.16	1.35	1.43
13	M	170	CLA	C1B-CHB	-4.15	1.35	1.43
13	L	158	CLA	C1B-CHB	-4.15	1.35	1.43
13	L	157	CLA	C1B-CHB	-4.15	1.35	1.43
13	J	179	CLA	C1B-CHB	-4.11	1.35	1.43
15	R	91	HEM	C3B-C2B	-4.06	1.42	1.52
15	I	88	HEM	C3B-C2B	-4.05	1.42	1.52
15	O	90	HEM	C3B-C2B	-4.04	1.42	1.52
15	F	50	HEM	C3B-C2B	-4.02	1.42	1.52
15	F	50	HEM	C4D-ND	-2.54	1.34	1.38
15	I	88	HEM	C4D-ND	-2.54	1.34	1.38
15	R	91	HEM	C4D-ND	-2.53	1.34	1.38
15	O	90	HEM	C4D-ND	-2.51	1.34	1.38
14	B	177	PHO	C1D-ND	-2.35	1.33	1.38
14	A	177	PHO	C1D-ND	-2.34	1.33	1.38
14	K	177	PHO	C1D-ND	-2.33	1.33	1.38
14	J	177	PHO	C1D-ND	-2.32	1.33	1.38
14	K	177	PHO	C4D-CHA	-2.29	1.38	1.45
14	J	177	PHO	C4D-CHA	-2.28	1.38	1.45
14	B	177	PHO	C4D-CHA	-2.27	1.39	1.45
14	A	177	PHO	C4D-CHA	-2.27	1.39	1.45
14	K	177	PHO	CHB-C1B	-2.22	1.34	1.39
14	B	177	PHO	CHB-C1B	-2.22	1.34	1.39
14	A	177	PHO	CHB-C1B	-2.19	1.34	1.39
14	J	177	PHO	CHB-C1B	-2.17	1.35	1.39
13	M	162	CLA	CAD-CBD	2.02	1.56	1.54
15	R	91	HEM	FE-NB	2.16	2.08	1.97
15	I	88	HEM	FE-NB	2.17	2.09	1.97
15	F	50	HEM	FE-NB	2.18	2.09	1.97
15	O	90	HEM	FE-NB	2.19	2.09	1.97
15	R	91	HEM	FE-NC	2.96	2.07	1.95
15	O	90	HEM	FE-NC	2.97	2.07	1.95
15	I	88	HEM	FE-NC	2.97	2.07	1.95
15	F	50	HEM	FE-NC	2.98	2.07	1.95
13	L	157	CLA	C2B-C1B	3.52	1.46	1.40
13	C	157	CLA	C2B-C1B	3.54	1.46	1.40
13	J	174	CLA	C2B-C1B	3.54	1.46	1.40
13	M	168	CLA	C2B-C1B	3.54	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	176	CLA	C2B-C1B	3.55	1.46	1.40
13	A	179	CLA	C2B-C1B	3.56	1.46	1.40
13	D	168	CLA	C2B-C1B	3.56	1.46	1.40
13	D	170	CLA	C2B-C1B	3.57	1.46	1.40
13	A	174	CLA	C2B-C1B	3.57	1.46	1.40
13	J	176	CLA	C2B-C1B	3.57	1.46	1.40
13	A	175	CLA	C2B-C1B	3.57	1.46	1.40
13	M	163	CLA	C2B-C1B	3.57	1.46	1.40
13	J	179	CLA	C2B-C1B	3.57	1.46	1.40
13	C	159	CLA	C2B-C1B	3.57	1.46	1.40
13	L	158	CLA	C2B-C1B	3.57	1.46	1.40
13	L	163	CLA	C2B-C1B	3.58	1.46	1.40
13	L	160	CLA	C2B-C1B	3.58	1.46	1.40
13	C	168	CLA	C2B-C1B	3.58	1.46	1.40
13	D	167	CLA	C2B-C1B	3.58	1.46	1.40
13	M	165	CLA	C2B-C1B	3.58	1.46	1.40
13	J	175	CLA	C2B-C1B	3.59	1.46	1.40
13	C	160	CLA	C2B-C1B	3.59	1.46	1.40
13	C	158	CLA	C2B-C1B	3.59	1.46	1.40
13	D	157	CLA	C2B-C1B	3.59	1.46	1.40
13	M	159	CLA	C2B-C1B	3.59	1.46	1.40
13	M	167	CLA	C2B-C1B	3.59	1.46	1.40
13	L	159	CLA	C2B-C1B	3.59	1.46	1.40
13	D	162	CLA	C2B-C1B	3.59	1.46	1.40
13	C	162	CLA	C2B-C1B	3.59	1.46	1.40
13	D	163	CLA	C2B-C1B	3.59	1.46	1.40
13	M	169	CLA	C2B-C1B	3.59	1.46	1.40
13	D	166	CLA	C2B-C1B	3.59	1.46	1.40
13	D	165	CLA	C2B-C1B	3.60	1.46	1.40
13	C	166	CLA	C2B-C1B	3.60	1.46	1.40
13	D	169	CLA	C2B-C1B	3.60	1.46	1.40
13	M	157	CLA	C2B-C1B	3.60	1.46	1.40
13	M	170	CLA	C2B-C1B	3.60	1.46	1.40
13	C	163	CLA	C2B-C1B	3.60	1.46	1.40
13	P	313	CLA	C2B-C1B	3.60	1.46	1.40
13	D	164	CLA	C2B-C1B	3.61	1.46	1.40
13	D	161	CLA	C2B-C1B	3.61	1.46	1.40
13	L	162	CLA	C2B-C1B	3.61	1.46	1.40
13	L	168	CLA	C2B-C1B	3.61	1.46	1.40
13	B	178	CLA	C2B-C1B	3.61	1.46	1.40
13	M	158	CLA	C2B-C1B	3.61	1.46	1.40
13	D	159	CLA	C2B-C1B	3.61	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	313	CLA	C2B-C1B	3.61	1.46	1.40
13	A	178	CLA	C2B-C1B	3.61	1.46	1.40
13	D	156	CLA	C2B-C1B	3.61	1.46	1.40
13	M	162	CLA	C2B-C1B	3.62	1.46	1.40
13	C	161	CLA	C2B-C1B	3.62	1.46	1.40
13	L	161	CLA	C2B-C1B	3.62	1.46	1.40
13	C	167	CLA	C2B-C1B	3.62	1.46	1.40
13	M	161	CLA	C2B-C1B	3.62	1.46	1.40
13	C	165	CLA	C2B-C1B	3.62	1.46	1.40
13	L	166	CLA	C2B-C1B	3.62	1.46	1.40
13	K	178	CLA	C2B-C1B	3.62	1.46	1.40
13	D	158	CLA	C2B-C1B	3.62	1.46	1.40
13	K	176	CLA	C2B-C1B	3.63	1.46	1.40
13	L	165	CLA	C2B-C1B	3.63	1.46	1.40
13	D	160	CLA	C2B-C1B	3.63	1.46	1.40
13	B	176	CLA	C2B-C1B	3.63	1.46	1.40
13	M	164	CLA	C2B-C1B	3.63	1.46	1.40
13	M	156	CLA	C2B-C1B	3.63	1.46	1.40
13	C	164	CLA	C2B-C1B	3.64	1.46	1.40
13	M	166	CLA	C2B-C1B	3.64	1.46	1.40
13	L	167	CLA	C2B-C1B	3.64	1.46	1.40
13	L	164	CLA	C2B-C1B	3.65	1.46	1.40
13	J	178	CLA	C2B-C1B	3.65	1.46	1.40
13	M	160	CLA	C2B-C1B	3.65	1.46	1.40
16	B	179	PL9	C3-C2	4.13	1.43	1.32
16	K	179	PL9	C3-C2	4.13	1.43	1.32
13	K	176	CLA	C3B-C4B	4.77	1.48	1.40
13	L	160	CLA	C3B-C4B	4.79	1.48	1.40
13	C	160	CLA	C3B-C4B	4.79	1.48	1.40
13	B	176	CLA	C3B-C4B	4.82	1.48	1.40
13	D	168	CLA	C3B-C4B	4.83	1.48	1.40
13	L	165	CLA	C3B-C4B	4.83	1.48	1.40
13	M	168	CLA	C3B-C4B	4.84	1.48	1.40
13	A	178	CLA	C3B-C4B	4.84	1.48	1.40
13	J	178	CLA	C3B-C4B	4.84	1.48	1.40
13	L	158	CLA	C3B-C4B	4.85	1.48	1.40
13	C	164	CLA	C3B-C4B	4.85	1.48	1.40
13	L	163	CLA	C3B-C4B	4.85	1.48	1.40
13	D	159	CLA	C3B-C4B	4.85	1.48	1.40
13	J	174	CLA	C3B-C4B	4.85	1.48	1.40
13	D	157	CLA	C3B-C4B	4.85	1.48	1.40
13	M	158	CLA	C3B-C4B	4.85	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	169	CLA	C3B-C4B	4.85	1.48	1.40
13	G	313	CLA	C3B-C4B	4.86	1.48	1.40
13	A	176	CLA	C3B-C4B	4.86	1.48	1.40
13	M	167	CLA	C3B-C4B	4.86	1.48	1.40
13	C	165	CLA	C3B-C4B	4.86	1.48	1.40
13	C	168	CLA	C3B-C4B	4.86	1.48	1.40
13	P	313	CLA	C3B-C4B	4.86	1.48	1.40
13	M	157	CLA	C3B-C4B	4.86	1.48	1.40
13	L	161	CLA	C3B-C4B	4.87	1.48	1.40
13	J	176	CLA	C3B-C4B	4.87	1.48	1.40
13	C	162	CLA	C3B-C4B	4.87	1.48	1.40
13	L	164	CLA	C3B-C4B	4.87	1.48	1.40
13	C	161	CLA	C3B-C4B	4.87	1.48	1.40
13	L	168	CLA	C3B-C4B	4.87	1.48	1.40
13	C	163	CLA	C3B-C4B	4.87	1.48	1.40
13	C	158	CLA	C3B-C4B	4.87	1.48	1.40
13	D	156	CLA	C3B-C4B	4.87	1.48	1.40
13	D	167	CLA	C3B-C4B	4.88	1.48	1.40
13	D	166	CLA	C3B-C4B	4.88	1.48	1.40
13	D	162	CLA	C3B-C4B	4.88	1.48	1.40
13	A	174	CLA	C3B-C4B	4.88	1.48	1.40
13	M	162	CLA	C3B-C4B	4.88	1.48	1.40
13	M	161	CLA	C3B-C4B	4.88	1.48	1.40
13	D	158	CLA	C3B-C4B	4.88	1.48	1.40
13	J	179	CLA	C3B-C4B	4.88	1.48	1.40
13	D	161	CLA	C3B-C4B	4.88	1.48	1.40
13	C	157	CLA	C3B-C4B	4.89	1.48	1.40
13	M	159	CLA	C3B-C4B	4.89	1.48	1.40
13	M	169	CLA	C3B-C4B	4.89	1.48	1.40
13	M	166	CLA	C3B-C4B	4.89	1.48	1.40
13	L	162	CLA	C3B-C4B	4.89	1.48	1.40
13	B	178	CLA	C3B-C4B	4.89	1.48	1.40
13	A	179	CLA	C3B-C4B	4.89	1.48	1.40
13	L	157	CLA	C3B-C4B	4.89	1.48	1.40
13	K	178	CLA	C3B-C4B	4.90	1.48	1.40
13	M	164	CLA	C3B-C4B	4.90	1.48	1.40
13	L	166	CLA	C3B-C4B	4.90	1.48	1.40
13	M	170	CLA	C3B-C4B	4.91	1.48	1.40
13	C	166	CLA	C3B-C4B	4.91	1.48	1.40
13	C	159	CLA	C3B-C4B	4.91	1.48	1.40
13	D	164	CLA	C3B-C4B	4.91	1.48	1.40
13	J	175	CLA	C3B-C4B	4.92	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	156	CLA	C3B-C4B	4.92	1.48	1.40
13	L	159	CLA	C3B-C4B	4.92	1.48	1.40
13	C	167	CLA	C3B-C4B	4.92	1.48	1.40
13	D	163	CLA	C3B-C4B	4.92	1.48	1.40
13	D	170	CLA	C3B-C4B	4.92	1.48	1.40
13	A	175	CLA	C3B-C4B	4.93	1.48	1.40
13	M	165	CLA	C3B-C4B	4.93	1.48	1.40
13	D	160	CLA	C3B-C4B	4.94	1.48	1.40
13	D	165	CLA	C3B-C4B	4.94	1.48	1.40
13	M	160	CLA	C3B-C4B	4.94	1.48	1.40
13	M	163	CLA	C3B-C4B	4.95	1.48	1.40
13	L	167	CLA	C3B-C4B	4.95	1.48	1.40
16	K	179	PL9	C6-C5	5.12	1.46	1.32
16	B	179	PL9	C6-C5	5.13	1.46	1.32
15	F	50	HEM	C3A-C4A	6.82	1.51	1.40
15	I	88	HEM	C3A-C4A	6.84	1.51	1.40
15	R	91	HEM	C3A-C4A	6.84	1.51	1.40
15	O	90	HEM	C3A-C4A	6.87	1.52	1.40
15	F	50	HEM	C2A-C1A	7.37	1.52	1.40
15	O	90	HEM	C2A-C1A	7.38	1.52	1.40
15	I	88	HEM	C2A-C1A	7.38	1.52	1.40
15	R	91	HEM	C2A-C1A	7.40	1.52	1.40

All (328) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	I	88	HEM	C3D-C4D-CHA	-7.15	116.84	124.06
15	R	91	HEM	C3D-C4D-CHA	-7.10	116.89	124.06
15	F	50	HEM	C3D-C4D-CHA	-7.05	116.95	124.06
15	O	90	HEM	C3D-C4D-CHA	-6.98	117.01	124.06
15	I	88	HEM	C2D-C3D-C4D	-5.11	98.78	103.90
15	R	91	HEM	C2D-C3D-C4D	-5.10	98.79	103.90
15	F	50	HEM	C2D-C3D-C4D	-5.02	98.87	103.90
15	O	90	HEM	C2D-C3D-C4D	-4.98	98.91	103.90
15	O	90	HEM	CHB-C1B-NB	-2.48	122.03	124.52
15	F	50	HEM	CHB-C1B-NB	-2.46	122.06	124.52
15	R	91	HEM	CHB-C1B-NB	-2.45	122.07	124.52
15	I	88	HEM	CHB-C1B-NB	-2.41	122.11	124.52
13	J	175	CLA	C3B-C4B-NB	-2.25	108.08	110.09
13	L	167	CLA	C3B-C4B-NB	-2.23	108.09	110.09
13	M	156	CLA	C3B-C4B-NB	-2.23	108.09	110.09
13	L	162	CLA	C3B-C4B-NB	-2.22	108.10	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	175	CLA	C3B-C4B-NB	-2.22	108.10	110.09
13	C	167	CLA	C3B-C4B-NB	-2.21	108.11	110.09
13	M	168	CLA	C3B-C4B-NB	-2.21	108.11	110.09
13	D	157	CLA	C3B-C4B-NB	-2.21	108.11	110.09
13	M	164	CLA	C3B-C4B-NB	-2.21	108.11	110.09
13	L	161	CLA	C3B-C4B-NB	-2.20	108.11	110.09
13	L	158	CLA	C3B-C4B-NB	-2.20	108.11	110.09
13	D	156	CLA	C3B-C4B-NB	-2.20	108.12	110.09
13	L	157	CLA	C3B-C4B-NB	-2.20	108.12	110.09
13	D	160	CLA	C3B-C4B-NB	-2.20	108.12	110.09
13	M	159	CLA	C3B-C4B-NB	-2.20	108.12	110.09
13	M	157	CLA	C3B-C4B-NB	-2.20	108.12	110.09
13	C	157	CLA	C3B-C4B-NB	-2.20	108.12	110.09
15	F	50	HEM	C3A-C2A-C1A	-2.19	104.37	106.29
13	C	158	CLA	C3B-C4B-NB	-2.19	108.13	110.09
13	M	161	CLA	C3B-C4B-NB	-2.19	108.13	110.09
13	C	164	CLA	C3B-C4B-NB	-2.19	108.13	110.09
13	D	168	CLA	C3B-C4B-NB	-2.19	108.13	110.09
13	L	164	CLA	C3B-C4B-NB	-2.18	108.13	110.09
13	D	161	CLA	C3B-C4B-NB	-2.18	108.13	110.09
13	C	162	CLA	C3B-C4B-NB	-2.18	108.13	110.09
13	J	176	CLA	C3B-C4B-NB	-2.18	108.13	110.09
13	C	161	CLA	C3B-C4B-NB	-2.18	108.14	110.09
13	D	159	CLA	C3B-C4B-NB	-2.18	108.14	110.09
15	R	91	HEM	C3A-C2A-C1A	-2.18	104.38	106.29
13	C	163	CLA	C3B-C4B-NB	-2.17	108.14	110.09
13	M	162	CLA	C3B-C4B-NB	-2.17	108.14	110.09
13	A	176	CLA	C3B-C4B-NB	-2.17	108.14	110.09
13	D	158	CLA	C3B-C4B-NB	-2.17	108.14	110.09
13	A	179	CLA	C3B-C4B-NB	-2.17	108.14	110.09
15	I	88	HEM	C3A-C2A-C1A	-2.17	104.39	106.29
13	D	164	CLA	C3B-C4B-NB	-2.17	108.15	110.09
15	O	90	HEM	C3A-C2A-C1A	-2.17	104.39	106.29
13	M	163	CLA	C3B-C4B-NB	-2.16	108.15	110.09
13	C	165	CLA	C3B-C4B-NB	-2.16	108.15	110.09
13	L	159	CLA	C3B-C4B-NB	-2.16	108.15	110.09
13	J	179	CLA	C3B-C4B-NB	-2.16	108.15	110.09
13	D	163	CLA	C3B-C4B-NB	-2.16	108.15	110.09
13	C	166	CLA	C3B-C4B-NB	-2.16	108.16	110.09
13	L	163	CLA	C3B-C4B-NB	-2.15	108.16	110.09
13	M	158	CLA	C3B-C4B-NB	-2.15	108.16	110.09
13	M	160	CLA	C3B-C4B-NB	-2.15	108.16	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	166	CLA	C3B-C4B-NB	-2.15	108.16	110.09
13	D	162	CLA	C3B-C4B-NB	-2.15	108.16	110.09
13	P	313	CLA	C3B-C4B-NB	-2.15	108.16	110.09
13	A	178	CLA	C3B-C4B-NB	-2.14	108.17	110.09
13	L	165	CLA	C3B-C4B-NB	-2.14	108.17	110.09
13	D	165	CLA	C3B-C4B-NB	-2.14	108.17	110.09
13	D	170	CLA	C3B-C4B-NB	-2.14	108.17	110.09
13	G	313	CLA	C3B-C4B-NB	-2.13	108.18	110.09
13	C	159	CLA	C3B-C4B-NB	-2.13	108.18	110.09
13	C	160	CLA	C3B-C4B-NB	-2.13	108.18	110.09
13	M	170	CLA	C3B-C4B-NB	-2.13	108.18	110.09
13	K	178	CLA	C3B-C4B-NB	-2.13	108.18	110.09
13	C	168	CLA	C3B-C4B-NB	-2.13	108.18	110.09
13	B	178	CLA	C3B-C4B-NB	-2.13	108.18	110.09
13	D	166	CLA	C3B-C4B-NB	-2.12	108.19	110.09
13	J	178	CLA	C3B-C4B-NB	-2.12	108.19	110.09
13	L	168	CLA	C3B-C4B-NB	-2.12	108.19	110.09
13	M	166	CLA	C3B-C4B-NB	-2.12	108.19	110.09
13	L	160	CLA	C3B-C4B-NB	-2.11	108.20	110.09
13	D	167	CLA	C3B-C4B-NB	-2.11	108.20	110.09
13	J	174	CLA	C3B-C4B-NB	-2.11	108.20	110.09
13	M	169	CLA	C3B-C4B-NB	-2.10	108.20	110.09
13	B	176	CLA	C3B-C4B-NB	-2.10	108.20	110.09
13	M	167	CLA	C3B-C4B-NB	-2.10	108.21	110.09
13	A	174	CLA	C3B-C4B-NB	-2.10	108.21	110.09
13	D	169	CLA	C3B-C4B-NB	-2.09	108.21	110.09
13	M	165	CLA	C3B-C4B-NB	-2.09	108.22	110.09
13	K	176	CLA	C3B-C4B-NB	-2.07	108.23	110.09
15	R	91	HEM	CHA-C4D-ND	2.26	126.78	124.52
15	O	90	HEM	CHA-C4D-ND	2.27	126.79	124.52
15	F	50	HEM	CHA-C4D-ND	2.31	126.83	124.52
15	I	88	HEM	CHA-C4D-ND	2.33	126.85	124.52
15	I	88	HEM	C2B-C1B-CHB	2.44	126.51	124.06
15	F	50	HEM	C2B-C1B-CHB	2.47	126.55	124.06
15	R	91	HEM	C2B-C1B-CHB	2.48	126.56	124.06
15	O	90	HEM	C2B-C1B-CHB	2.52	126.60	124.06
13	L	160	CLA	C2A-C1A-CHA	2.64	126.44	122.80
13	L	167	CLA	C2A-C1A-CHA	2.65	126.46	122.80
13	C	159	CLA	C2A-C1A-CHA	2.65	126.46	122.80
13	L	161	CLA	C2A-C1A-CHA	2.65	126.47	122.80
13	L	158	CLA	C2A-C1A-CHA	2.66	126.47	122.80
13	L	159	CLA	C2A-C1A-CHA	2.66	126.48	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	K	176	CLA	C2A-C1A-CHA	2.66	126.48	122.80
13	J	179	CLA	C2A-C1A-CHA	2.66	126.48	122.80
13	D	168	CLA	C2A-C1A-CHA	2.67	126.48	122.80
13	J	178	CLA	C2A-C1A-CHA	2.67	126.48	122.80
13	M	160	CLA	C2A-C1A-CHA	2.67	126.49	122.80
13	M	170	CLA	C2A-C1A-CHA	2.67	126.49	122.80
13	D	160	CLA	C2A-C1A-CHA	2.67	126.49	122.80
13	C	163	CLA	C2A-C1A-CHA	2.67	126.49	122.80
13	C	168	CLA	C2A-C1A-CHA	2.67	126.49	122.80
13	C	160	CLA	C2A-C1A-CHA	2.68	126.50	122.80
13	M	158	CLA	C2A-C1A-CHA	2.68	126.50	122.80
13	C	162	CLA	C2A-C1A-CHA	2.68	126.50	122.80
13	M	163	CLA	C2A-C1A-CHA	2.68	126.50	122.80
13	D	158	CLA	C2A-C1A-CHA	2.68	126.50	122.80
13	C	167	CLA	C2A-C1A-CHA	2.68	126.50	122.80
13	M	167	CLA	C2A-C1A-CHA	2.68	126.51	122.80
13	L	168	CLA	C2A-C1A-CHA	2.68	126.51	122.80
13	D	164	CLA	C2A-C1A-CHA	2.68	126.51	122.80
13	A	178	CLA	C2A-C1A-CHA	2.68	126.51	122.80
13	C	165	CLA	C2A-C1A-CHA	2.68	126.51	122.80
13	B	176	CLA	C2A-C1A-CHA	2.69	126.51	122.80
13	L	163	CLA	C2A-C1A-CHA	2.69	126.51	122.80
13	L	162	CLA	C2A-C1A-CHA	2.69	126.51	122.80
13	M	165	CLA	C2A-C1A-CHA	2.69	126.51	122.80
13	D	166	CLA	C2A-C1A-CHA	2.69	126.52	122.80
13	A	179	CLA	C2A-C1A-CHA	2.69	126.52	122.80
13	J	176	CLA	C2A-C1A-CHA	2.69	126.52	122.80
13	D	157	CLA	C2A-C1A-CHA	2.69	126.52	122.80
13	D	163	CLA	C2A-C1A-CHA	2.69	126.52	122.80
13	A	175	CLA	C2A-C1A-CHA	2.69	126.52	122.80
13	M	169	CLA	C2A-C1A-CHA	2.69	126.52	122.80
13	M	166	CLA	C2A-C1A-CHA	2.69	126.52	122.80
13	C	161	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	C	158	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	J	175	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	D	165	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	M	157	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	M	164	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	M	168	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	D	170	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	P	313	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	B	178	CLA	C2A-C1A-CHA	2.70	126.53	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	162	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	L	164	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	D	167	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	A	176	CLA	C2A-C1A-CHA	2.70	126.53	122.80
13	M	161	CLA	C2A-C1A-CHA	2.70	126.54	122.80
13	D	169	CLA	C2A-C1A-CHA	2.71	126.54	122.80
13	C	157	CLA	C2A-C1A-CHA	2.71	126.54	122.80
13	D	162	CLA	C2A-C1A-CHA	2.71	126.54	122.80
13	D	161	CLA	C2A-C1A-CHA	2.71	126.54	122.80
13	L	157	CLA	C2A-C1A-CHA	2.71	126.54	122.80
13	K	178	CLA	C2A-C1A-CHA	2.71	126.54	122.80
13	D	156	CLA	C2A-C1A-CHA	2.71	126.55	122.80
13	D	159	CLA	C2A-C1A-CHA	2.71	126.55	122.80
13	C	166	CLA	C2A-C1A-CHA	2.72	126.55	122.80
13	G	313	CLA	C2A-C1A-CHA	2.72	126.56	122.80
13	M	156	CLA	C2A-C1A-CHA	2.72	126.56	122.80
13	C	164	CLA	C2A-C1A-CHA	2.73	126.57	122.80
13	M	159	CLA	C2A-C1A-CHA	2.73	126.58	122.80
13	A	174	CLA	C2A-C1A-CHA	2.73	126.58	122.80
13	J	174	CLA	C2A-C1A-CHA	2.74	126.59	122.80
13	L	165	CLA	C2A-C1A-CHA	2.75	126.59	122.80
13	L	166	CLA	C2A-C1A-CHA	2.75	126.60	122.80
15	F	50	HEM	C3B-C2B-C1B	2.84	106.75	103.90
15	O	90	HEM	C3B-C2B-C1B	2.86	106.77	103.90
15	I	88	HEM	C3B-C2B-C1B	2.89	106.79	103.90
15	R	91	HEM	C3B-C2B-C1B	2.90	106.80	103.90
15	O	90	HEM	C3D-C4D-ND	2.96	116.20	110.17
15	F	50	HEM	C3D-C4D-ND	2.97	116.23	110.17
14	K	177	PHO	C4A-NA-C1A	2.97	111.29	108.36
14	B	177	PHO	C4A-NA-C1A	2.99	111.31	108.36
15	I	88	HEM	C3D-C4D-ND	3.01	116.30	110.17
15	R	91	HEM	C3D-C4D-ND	3.02	116.33	110.17
14	A	177	PHO	C4A-NA-C1A	3.05	111.36	108.36
14	J	177	PHO	C4A-NA-C1A	3.08	111.40	108.36
15	F	50	HEM	C3B-C4B-CHC	3.15	128.15	122.58
15	O	90	HEM	C3B-C4B-CHC	3.15	128.15	122.58
15	I	88	HEM	C3B-C4B-CHC	3.25	128.33	122.58
15	R	91	HEM	C3B-C4B-CHC	3.26	128.35	122.58
14	B	177	PHO	CBD-CHA-C1A	3.45	131.17	125.34
14	A	177	PHO	CBD-CHA-C1A	3.46	131.17	125.34
14	K	177	PHO	CBD-CHA-C1A	3.46	131.18	125.34
14	J	177	PHO	CBD-CHA-C1A	3.46	131.18	125.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	164	CLA	CBD-CAD-C3D	3.83	107.09	104.39
13	C	164	CLA	CBD-CAD-C3D	3.84	107.10	104.39
13	D	162	CLA	CBD-CAD-C3D	3.85	107.11	104.39
13	C	159	CLA	CBD-CAD-C3D	3.88	107.13	104.39
13	L	159	CLA	CBD-CAD-C3D	3.88	107.13	104.39
13	K	176	CLA	CBD-CAD-C3D	3.88	107.13	104.39
13	M	157	CLA	CBD-CAD-C3D	3.89	107.14	104.39
13	K	178	CLA	CBD-CAD-C3D	3.89	107.14	104.39
13	J	176	CLA	CBD-CAD-C3D	3.89	107.14	104.39
13	M	164	CLA	CBD-CAD-C3D	3.90	107.14	104.39
13	M	162	CLA	CBD-CAD-C3D	3.90	107.14	104.39
13	M	169	CLA	CBD-CAD-C3D	3.90	107.14	104.39
13	L	166	CLA	CBD-CAD-C3D	3.90	107.15	104.39
13	L	158	CLA	CBD-CAD-C3D	3.91	107.15	104.39
13	C	160	CLA	CBD-CAD-C3D	3.91	107.15	104.39
13	D	164	CLA	CBD-CAD-C3D	3.92	107.16	104.39
13	M	159	CLA	CBD-CAD-C3D	3.93	107.16	104.39
13	D	157	CLA	CBD-CAD-C3D	3.93	107.16	104.39
13	B	176	CLA	CBD-CAD-C3D	3.93	107.16	104.39
13	C	158	CLA	CBD-CAD-C3D	3.93	107.17	104.39
13	B	178	CLA	CBD-CAD-C3D	3.93	107.17	104.39
13	D	158	CLA	CBD-CAD-C3D	3.93	107.17	104.39
13	M	158	CLA	CBD-CAD-C3D	3.93	107.17	104.39
13	A	176	CLA	CBD-CAD-C3D	3.94	107.17	104.39
13	C	166	CLA	CBD-CAD-C3D	3.94	107.17	104.39
13	M	166	CLA	CBD-CAD-C3D	3.94	107.17	104.39
13	J	175	CLA	CBD-CAD-C3D	3.95	107.18	104.39
13	D	166	CLA	CBD-CAD-C3D	3.95	107.18	104.39
13	D	159	CLA	CBD-CAD-C3D	3.95	107.18	104.39
13	D	169	CLA	CBD-CAD-C3D	3.96	107.18	104.39
13	L	160	CLA	CBD-CAD-C3D	3.96	107.19	104.39
13	L	161	CLA	CBD-CAD-C3D	3.96	107.19	104.39
13	C	162	CLA	CBD-CAD-C3D	3.96	107.19	104.39
13	A	175	CLA	CBD-CAD-C3D	3.97	107.19	104.39
13	P	313	CLA	CBD-CAD-C3D	3.97	107.20	104.39
13	A	178	CLA	CBD-CAD-C3D	3.98	107.20	104.39
13	D	167	CLA	CBD-CAD-C3D	3.98	107.20	104.39
13	M	167	CLA	CBD-CAD-C3D	3.98	107.20	104.39
13	J	178	CLA	CBD-CAD-C3D	3.98	107.20	104.39
13	C	163	CLA	CBD-CAD-C3D	3.98	107.20	104.39
13	L	162	CLA	CBD-CAD-C3D	3.98	107.20	104.39
13	D	163	CLA	CBD-CAD-C3D	3.99	107.20	104.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	163	CLA	CBD-CAD-C3D	3.99	107.21	104.39
13	C	161	CLA	CBD-CAD-C3D	4.00	107.21	104.39
13	M	168	CLA	CBD-CAD-C3D	4.00	107.21	104.39
13	D	168	CLA	CBD-CAD-C3D	4.00	107.22	104.39
13	C	157	CLA	CBD-CAD-C3D	4.00	107.22	104.39
13	G	313	CLA	CBD-CAD-C3D	4.01	107.22	104.39
13	M	170	CLA	CBD-CAD-C3D	4.01	107.22	104.39
13	J	174	CLA	CBD-CAD-C3D	4.01	107.22	104.39
13	D	165	CLA	CBD-CAD-C3D	4.01	107.22	104.39
13	M	165	CLA	CBD-CAD-C3D	4.01	107.22	104.39
13	D	160	CLA	CBD-CAD-C3D	4.01	107.22	104.39
13	D	156	CLA	CBD-CAD-C3D	4.02	107.22	104.39
13	D	161	CLA	CBD-CAD-C3D	4.02	107.23	104.39
13	L	168	CLA	CBD-CAD-C3D	4.02	107.23	104.39
13	C	165	CLA	CBD-CAD-C3D	4.02	107.23	104.39
13	D	170	CLA	CBD-CAD-C3D	4.03	107.23	104.39
13	L	157	CLA	CBD-CAD-C3D	4.03	107.23	104.39
13	M	160	CLA	CBD-CAD-C3D	4.03	107.23	104.39
13	M	161	CLA	CBD-CAD-C3D	4.03	107.23	104.39
13	L	165	CLA	CBD-CAD-C3D	4.03	107.23	104.39
13	M	163	CLA	CBD-CAD-C3D	4.03	107.24	104.39
13	M	156	CLA	CBD-CAD-C3D	4.03	107.24	104.39
13	C	167	CLA	CBD-CAD-C3D	4.04	107.24	104.39
13	A	179	CLA	CBD-CAD-C3D	4.04	107.24	104.39
13	C	168	CLA	CBD-CAD-C3D	4.04	107.25	104.39
13	A	174	CLA	CBD-CAD-C3D	4.05	107.25	104.39
13	J	179	CLA	CBD-CAD-C3D	4.07	107.27	104.39
13	L	167	CLA	CBD-CAD-C3D	4.09	107.28	104.39
13	L	164	CLA	CAD-C3D-C2D	4.93	144.75	132.80
13	L	166	CLA	CAD-C3D-C2D	4.93	144.76	132.80
13	C	164	CLA	CAD-C3D-C2D	4.93	144.77	132.80
13	L	158	CLA	CAD-C3D-C2D	4.94	144.79	132.80
13	C	160	CLA	CAD-C3D-C2D	4.94	144.80	132.80
13	C	166	CLA	CAD-C3D-C2D	4.94	144.80	132.80
13	M	159	CLA	CAD-C3D-C2D	4.94	144.80	132.80
13	L	162	CLA	CAD-C3D-C2D	4.95	144.80	132.80
13	C	159	CLA	CAD-C3D-C2D	4.95	144.80	132.80
13	A	175	CLA	CAD-C3D-C2D	4.95	144.80	132.80
13	D	162	CLA	CAD-C3D-C2D	4.95	144.80	132.80
13	J	175	CLA	CAD-C3D-C2D	4.95	144.81	132.80
13	K	178	CLA	CAD-C3D-C2D	4.95	144.81	132.80
13	M	158	CLA	CAD-C3D-C2D	4.95	144.81	132.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	D	158	CLA	CAD-C3D-C2D	4.95	144.82	132.80
13	K	176	CLA	CAD-C3D-C2D	4.95	144.82	132.80
13	D	164	CLA	CAD-C3D-C2D	4.95	144.82	132.80
13	D	159	CLA	CAD-C3D-C2D	4.95	144.82	132.80
13	L	160	CLA	CAD-C3D-C2D	4.95	144.82	132.80
13	L	159	CLA	CAD-C3D-C2D	4.96	144.83	132.80
13	C	158	CLA	CAD-C3D-C2D	4.96	144.83	132.80
13	M	157	CLA	CAD-C3D-C2D	4.96	144.83	132.80
13	B	178	CLA	CAD-C3D-C2D	4.96	144.83	132.80
13	M	161	CLA	CAD-C3D-C2D	4.96	144.84	132.80
13	M	166	CLA	CAD-C3D-C2D	4.96	144.84	132.80
13	C	162	CLA	CAD-C3D-C2D	4.96	144.84	132.80
13	M	164	CLA	CAD-C3D-C2D	4.96	144.84	132.80
13	M	162	CLA	CAD-C3D-C2D	4.96	144.84	132.80
13	C	161	CLA	CAD-C3D-C2D	4.96	144.84	132.80
13	M	169	CLA	CAD-C3D-C2D	4.96	144.85	132.80
13	C	167	CLA	CAD-C3D-C2D	4.96	144.85	132.80
13	D	157	CLA	CAD-C3D-C2D	4.96	144.85	132.80
13	B	176	CLA	CAD-C3D-C2D	4.96	144.85	132.80
13	A	178	CLA	CAD-C3D-C2D	4.96	144.85	132.80
13	M	168	CLA	CAD-C3D-C2D	4.96	144.85	132.80
13	D	166	CLA	CAD-C3D-C2D	4.96	144.85	132.80
13	J	174	CLA	CAD-C3D-C2D	4.97	144.85	132.80
13	A	176	CLA	CAD-C3D-C2D	4.97	144.85	132.80
13	D	169	CLA	CAD-C3D-C2D	4.97	144.85	132.80
13	D	161	CLA	CAD-C3D-C2D	4.97	144.85	132.80
13	J	176	CLA	CAD-C3D-C2D	4.97	144.86	132.80
13	L	165	CLA	CAD-C3D-C2D	4.97	144.86	132.80
13	D	167	CLA	CAD-C3D-C2D	4.97	144.86	132.80
13	M	167	CLA	CAD-C3D-C2D	4.97	144.87	132.80
13	J	178	CLA	CAD-C3D-C2D	4.97	144.87	132.80
13	D	168	CLA	CAD-C3D-C2D	4.97	144.87	132.80
13	G	313	CLA	CAD-C3D-C2D	4.97	144.87	132.80
13	M	156	CLA	CAD-C3D-C2D	4.97	144.87	132.80
13	L	161	CLA	CAD-C3D-C2D	4.97	144.87	132.80
13	D	160	CLA	CAD-C3D-C2D	4.98	144.88	132.80
13	L	167	CLA	CAD-C3D-C2D	4.98	144.88	132.80
13	L	163	CLA	CAD-C3D-C2D	4.98	144.88	132.80
13	C	157	CLA	CAD-C3D-C2D	4.98	144.88	132.80
13	L	168	CLA	CAD-C3D-C2D	4.98	144.88	132.80
13	L	157	CLA	CAD-C3D-C2D	4.98	144.88	132.80
13	D	156	CLA	CAD-C3D-C2D	4.98	144.88	132.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	163	CLA	CAD-C3D-C2D	4.98	144.88	132.80
13	D	163	CLA	CAD-C3D-C2D	4.98	144.89	132.80
13	C	165	CLA	CAD-C3D-C2D	4.98	144.89	132.80
13	C	168	CLA	CAD-C3D-C2D	4.98	144.89	132.80
13	A	174	CLA	CAD-C3D-C2D	4.98	144.89	132.80
13	P	313	CLA	CAD-C3D-C2D	4.98	144.90	132.80
13	D	165	CLA	CAD-C3D-C2D	4.99	144.91	132.80
13	M	165	CLA	CAD-C3D-C2D	4.99	144.91	132.80
13	A	179	CLA	CAD-C3D-C2D	4.99	144.91	132.80
13	M	160	CLA	CAD-C3D-C2D	4.99	144.92	132.80
13	M	163	CLA	CAD-C3D-C2D	5.00	144.93	132.80
13	M	170	CLA	CAD-C3D-C2D	5.00	144.94	132.80
13	D	170	CLA	CAD-C3D-C2D	5.00	144.95	132.80
13	J	179	CLA	CAD-C3D-C2D	5.00	144.95	132.80
15	O	90	HEM	C3D-C2D-C1D	7.31	111.23	103.90
15	F	50	HEM	C3D-C2D-C1D	7.35	111.26	103.90
15	I	88	HEM	C3D-C2D-C1D	7.48	111.40	103.90
15	R	91	HEM	C3D-C2D-C1D	7.49	111.41	103.90

All (210) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	C	163	CLA	NC
13	C	163	CLA	ND
13	C	163	CLA	NA
13	C	166	CLA	NC
13	C	166	CLA	ND
13	C	166	CLA	NA
13	M	159	CLA	NC
13	M	159	CLA	ND
13	M	159	CLA	NA
13	C	159	CLA	NC
13	C	159	CLA	ND
13	C	159	CLA	NA
13	B	178	CLA	NC
13	B	178	CLA	ND
13	B	178	CLA	NA
13	D	160	CLA	NC
13	D	160	CLA	ND
13	D	160	CLA	NA
13	K	176	CLA	NC
13	K	176	CLA	ND

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Mol	Chain	Res	Type	Atom
13	K	176	CLA	NA
13	A	175	CLA	NC
13	A	175	CLA	ND
13	A	175	CLA	NA
13	D	164	CLA	NC
13	D	164	CLA	ND
13	D	164	CLA	NA
13	M	169	CLA	NC
13	M	169	CLA	ND
13	M	169	CLA	NA
13	L	161	CLA	NC
13	L	161	CLA	ND
13	L	161	CLA	NA
13	C	160	CLA	NC
13	C	160	CLA	ND
13	C	160	CLA	NA
13	L	159	CLA	NC
13	L	159	CLA	ND
13	L	159	CLA	NA
13	D	159	CLA	NC
13	D	159	CLA	ND
13	D	159	CLA	NA
13	D	156	CLA	NC
13	D	156	CLA	ND
13	D	156	CLA	NA
13	M	160	CLA	NC
13	M	160	CLA	ND
13	M	160	CLA	NA
13	M	158	CLA	NC
13	M	158	CLA	ND
13	M	158	CLA	NA
13	C	164	CLA	NC
13	C	164	CLA	ND
13	C	164	CLA	NA
13	L	166	CLA	NC
13	L	166	CLA	ND
13	L	166	CLA	NA
13	D	162	CLA	NC
13	D	162	CLA	ND
13	D	162	CLA	NA
13	K	178	CLA	NC
13	K	178	CLA	ND

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Mol	Chain	Res	Type	Atom
13	K	178	CLA	NA
13	J	175	CLA	NC
13	J	175	CLA	ND
13	J	175	CLA	NA
13	A	178	CLA	NC
13	A	178	CLA	ND
13	A	178	CLA	NA
13	M	162	CLA	NC
13	M	162	CLA	ND
13	M	162	CLA	NA
13	L	167	CLA	NC
13	L	167	CLA	ND
13	L	167	CLA	NA
13	C	157	CLA	NC
13	C	157	CLA	ND
13	C	157	CLA	NA
13	D	167	CLA	NC
13	D	167	CLA	ND
13	D	167	CLA	NA
13	L	160	CLA	NC
13	L	160	CLA	ND
13	L	160	CLA	NA
13	M	167	CLA	NC
13	M	167	CLA	ND
13	M	167	CLA	NA
13	D	166	CLA	NC
13	D	166	CLA	ND
13	D	166	CLA	NA
13	D	169	CLA	NC
13	D	169	CLA	ND
13	D	169	CLA	NA
13	M	161	CLA	NC
13	M	161	CLA	ND
13	M	161	CLA	NA
13	L	163	CLA	NC
13	L	163	CLA	ND
13	L	163	CLA	NA
13	M	163	CLA	NC
13	M	163	CLA	ND
13	M	163	CLA	NA
13	C	158	CLA	NC
13	C	158	CLA	ND

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Mol	Chain	Res	Type	Atom
13	C	158	CLA	NA
13	D	158	CLA	NC
13	D	158	CLA	ND
13	D	158	CLA	NA
13	L	164	CLA	NC
13	L	164	CLA	ND
13	L	164	CLA	NA
13	C	168	CLA	NC
13	C	168	CLA	ND
13	C	168	CLA	NA
13	L	165	CLA	NC
13	L	165	CLA	ND
13	L	165	CLA	NA
13	D	165	CLA	NC
13	D	165	CLA	ND
13	D	165	CLA	NA
13	C	162	CLA	NC
13	C	162	CLA	ND
13	C	162	CLA	NA
13	J	174	CLA	NC
13	J	174	CLA	ND
13	J	174	CLA	NA
13	G	313	CLA	NC
13	G	313	CLA	ND
13	G	313	CLA	NA
13	A	176	CLA	NC
13	A	176	CLA	ND
13	A	176	CLA	NA
13	M	170	CLA	NC
13	M	170	CLA	ND
13	M	170	CLA	NA
13	M	157	CLA	NC
13	M	157	CLA	ND
13	M	157	CLA	NA
13	D	161	CLA	NC
13	D	161	CLA	ND
13	D	161	CLA	NA
13	D	157	CLA	NC
13	D	157	CLA	ND
13	D	157	CLA	NA
13	J	178	CLA	NC
13	J	178	CLA	ND

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Mol	Chain	Res	Type	Atom
13	J	178	CLA	NA
13	L	158	CLA	NC
13	L	158	CLA	ND
13	L	158	CLA	NA
13	D	168	CLA	NC
13	D	168	CLA	ND
13	D	168	CLA	NA
13	L	168	CLA	NC
13	L	168	CLA	ND
13	L	168	CLA	NA
13	J	176	CLA	NC
13	J	176	CLA	ND
13	J	176	CLA	NA
13	C	161	CLA	NC
13	C	161	CLA	ND
13	C	161	CLA	NA
13	M	166	CLA	NC
13	M	166	CLA	ND
13	M	166	CLA	NA
13	D	170	CLA	NC
13	D	170	CLA	ND
13	D	170	CLA	NA
13	A	174	CLA	NC
13	A	174	CLA	ND
13	A	174	CLA	NA
13	C	167	CLA	NC
13	C	167	CLA	ND
13	C	167	CLA	NA
13	B	176	CLA	NC
13	B	176	CLA	ND
13	B	176	CLA	NA
13	J	179	CLA	NC
13	J	179	CLA	ND
13	J	179	CLA	NA
13	L	162	CLA	NC
13	L	162	CLA	ND
13	L	162	CLA	NA
13	M	164	CLA	NC
13	M	164	CLA	ND
13	M	164	CLA	NA
13	M	156	CLA	NC
13	M	156	CLA	ND

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Mol	Chain	Res	Type	Atom
13	M	156	CLA	NA
13	D	163	CLA	NC
13	D	163	CLA	ND
13	D	163	CLA	NA
13	M	168	CLA	NC
13	M	168	CLA	ND
13	M	168	CLA	NA
13	P	313	CLA	NC
13	P	313	CLA	ND
13	P	313	CLA	NA
13	A	179	CLA	NC
13	A	179	CLA	ND
13	A	179	CLA	NA
13	M	165	CLA	NC
13	M	165	CLA	ND
13	M	165	CLA	NA
13	L	157	CLA	NC
13	L	157	CLA	ND
13	L	157	CLA	NA
13	C	165	CLA	NC
13	C	165	CLA	ND
13	C	165	CLA	NA

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	168	CLA	2	0
13	D	165	CLA	3	0
13	D	168	CLA	4	0
13	G	313	CLA	4	0
13	L	168	CLA	2	0
13	M	165	CLA	3	0
13	M	168	CLA	4	0
13	P	313	CLA	4	0

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.