



# wwPDB X-ray Structure Validation Summary Report ⓘ

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

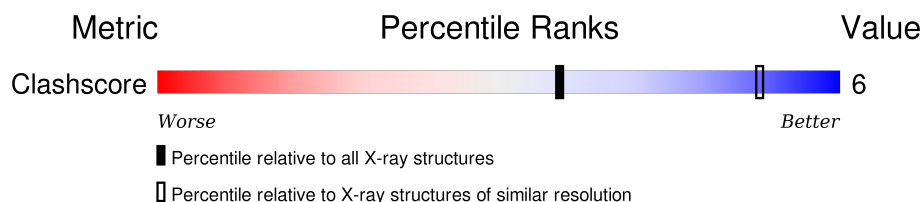
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

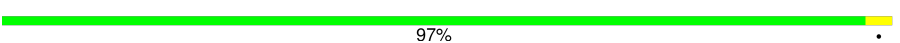
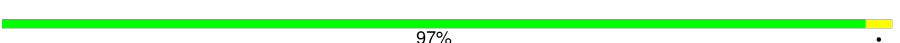



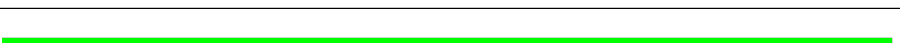
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1458 (4.10-3.50)

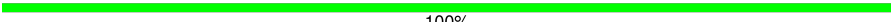
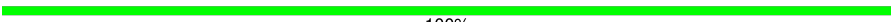






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	0	0
			4	4		

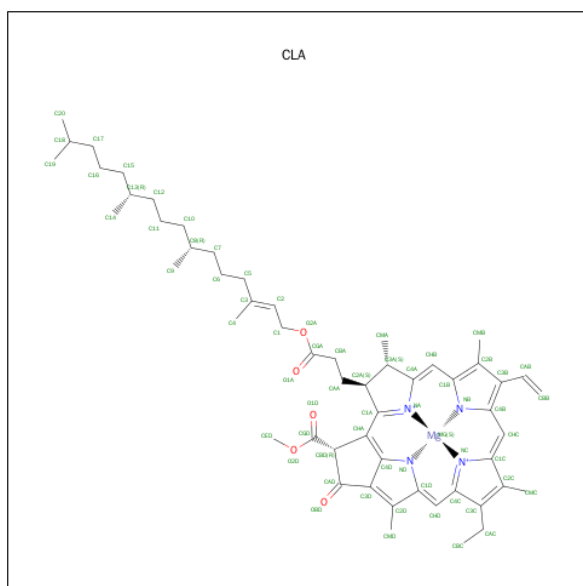
- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

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

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

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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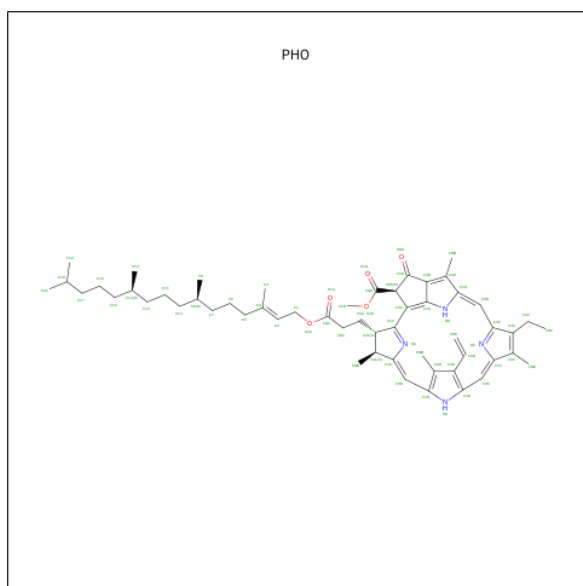
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	J	1	Total	C	Mg	N	0	0
			27	22	1	4		
13	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
13	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
13	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
13	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
13	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
13	L	1	Total	C	Mg	N	0	0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

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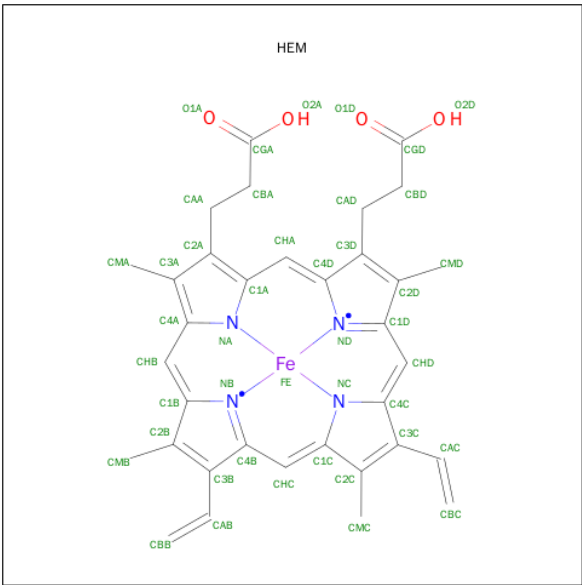
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
13	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
13	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
13	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
13	M	1	Total	C	Mg	N	0	0
			27	22	1	4		

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



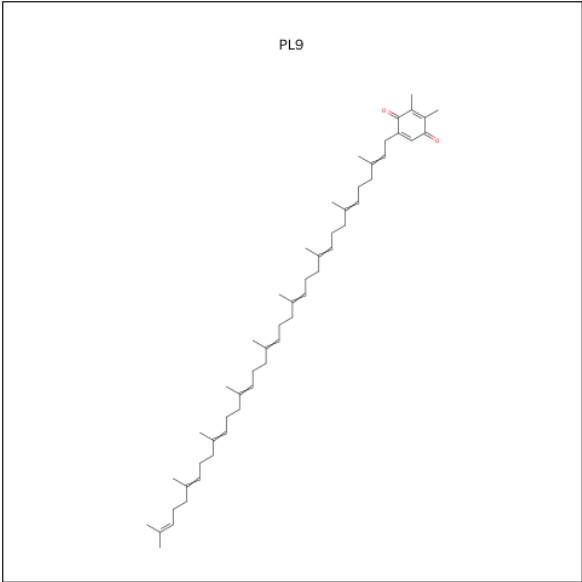
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	C	N	0	0
			26	22	4		
14	A	1	Total	C	N	0	0
			26	22	4		
14	K	1	Total	C	N	0	0
			26	22	4		
14	J	1	Total	C	N	0	0
			26	22	4		

- 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<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



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

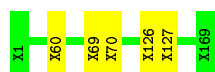
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

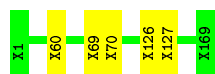
- Molecule 1: PHOTOSYSTEM II: SUBUNIT PSBA

Chain A:  97% .



- Molecule 1: PHOTOSYSTEM II: SUBUNIT PSBA

Chain J:  97% .



- Molecule 2: PHOTOSYSTEM II: SUBUNIT PSBD

Chain B:  97% .



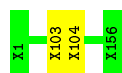
- Molecule 2: PHOTOSYSTEM II: SUBUNIT PSBD

Chain K:  97% .



- Molecule 3: PHOTOSYSTEM II: SUBUNIT PSBC

Chain C:  99% .



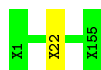
- Molecule 3: PHOTOSYSTEM II: SUBUNIT PSBC

Chain L:  99% .



- Molecule 4: PHOTOSYSTEM II: SUBUNIT PSBB

Chain D:  99%



- Molecule 4: PHOTOSYSTEM II: SUBUNIT PSBB

Chain M:  99%



- Molecule 5: PHOTOSYSTEM II: SUBUNIT PSBE

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: PHOTOSYSTEM II: SUBUNIT PSBE

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PHOTOSYSTEM II: SUBUNIT PSBF

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PHOTOSYSTEM II: SUBUNIT PSBF

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PHOTOSYSTEM II: SUBUNIT UNKNOWN

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PHOTOSYSTEM II: SUBUNIT UNKNOWN

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PHOTOSYSTEM II: SUBUNIT PSBO



Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PHOTOSYSTEM II: SUBUNIT PSBO

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PHOTOSYSTEM II: SUBUNIT PSBV

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PHOTOSYSTEM II: SUBUNIT PSBV

Chain R:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	1.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 [i](#)

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.

The worst 5 of 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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

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%)

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

The worst 5 of 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

The worst 5 of 328 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	88	HEM	C3D-C4D-CHA	-7.15	116.84	124.06

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

5 of 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

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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.