



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:44 PM GMT

PDB ID : 1YF6  
Title : Structure of a quintuple mutant of photosynthetic reaction center from rhodobacter sphaeroides  
Authors : Paddock, M.L.; Chang, C.; Xu, Q.; Abresch, E.C.; Axelrod, H.L.  
Deposited on : 2004-12-30  
Resolution : 2.25 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.

---

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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

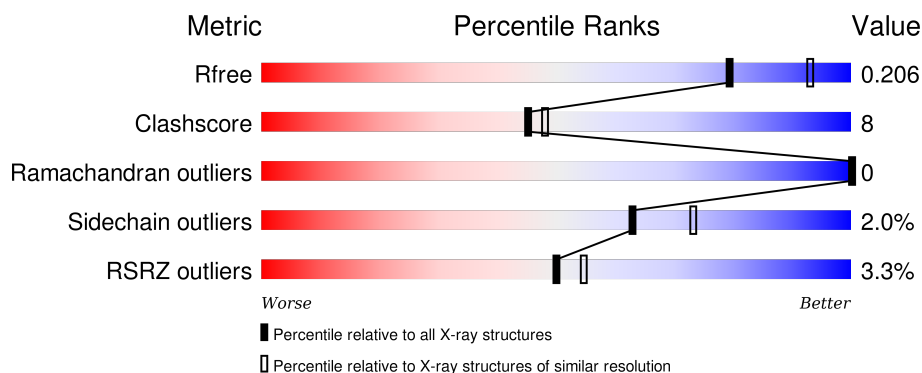
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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.

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	M	307	<div> <div>5%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
3	H	260	<div> <div>2%</div> <div>78%</div> <div>13%</div> <div>8%</div> </div>

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
11	CDL	M	862	-	-	-	X
12	HTO	L	863	-	-	-	X
13	LDA	L	864	-	-	-	X
13	LDA	L	865	-	-	-	X
13	LDA	M	866	-	-	-	X
14	GOL	L	869	-	X	-	X
7	BCL	L	852	X	-	-	-
7	BCL	L	854	X	-	-	-
7	BCL	M	851	X	-	-	-
7	BCL	M	853	X	-	-	-
7	BCL	M	856	X	-	-	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7450 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2233	1507	355	363	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	181	TYR	PHE	ENGINEERED	UNP P02954

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2418	1615	396	397	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	203	ASP	GLY	ENGINEERED	UNP P02953
M	210	PHE	TYR	ENGINEERED	UNP P02953
M	214	HIS	LEU	ENGINEERED	UNP P02953
M	260	TRP	ALA	ENGINEERED	UNP P02953

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	0	0
			1814	1160	311	334	9			

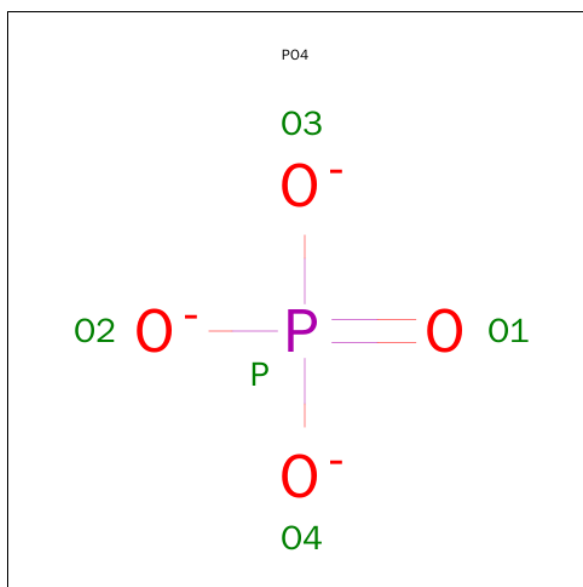
- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

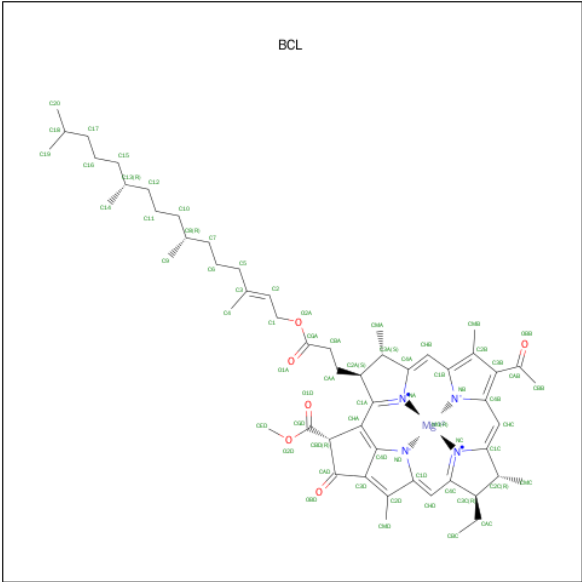
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



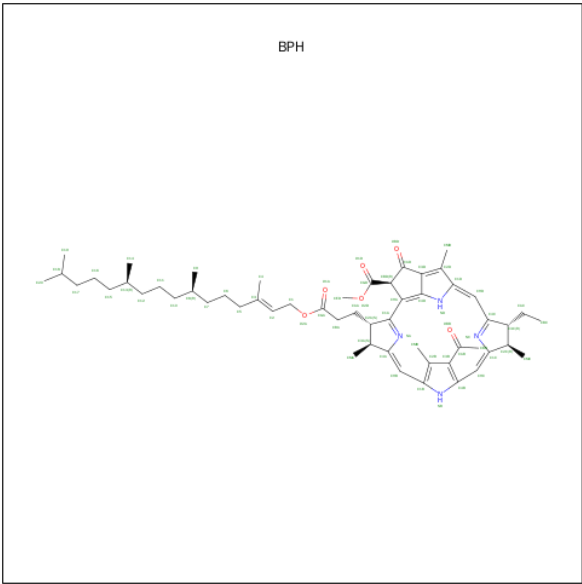
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	O	P	0	0
			5	4	1		
6	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



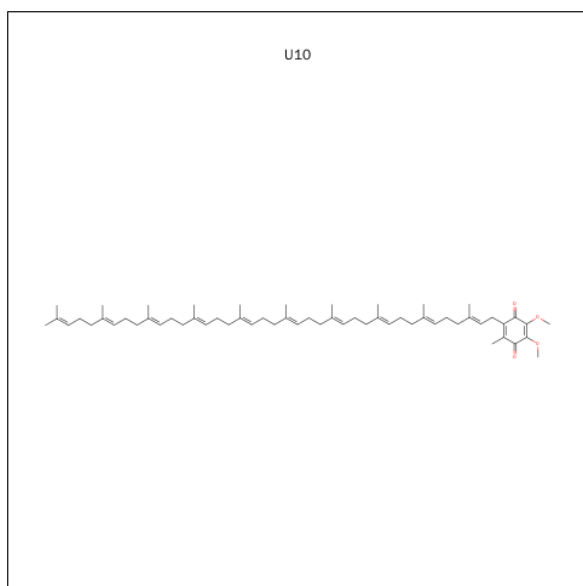
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



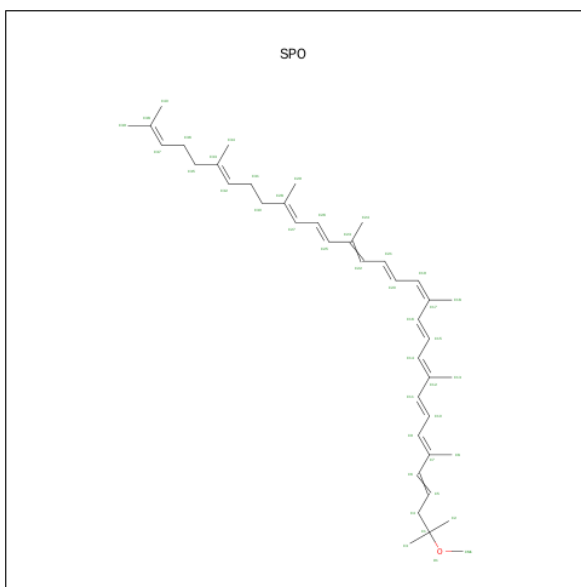
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			51	41	4	6		

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



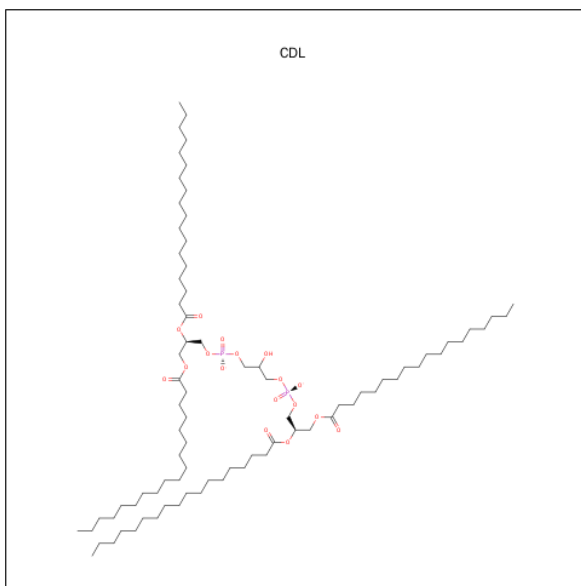
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			15	11	4		
9	L	1	Total	C	O	0	0
			16	12	4		
9	L	1	Total	C	O	0	0
			15	11	4		

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			42	41	1		

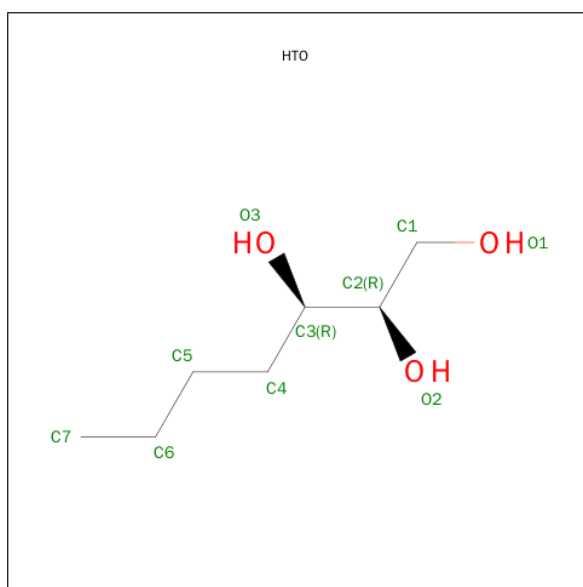
- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			81	62	17	2		

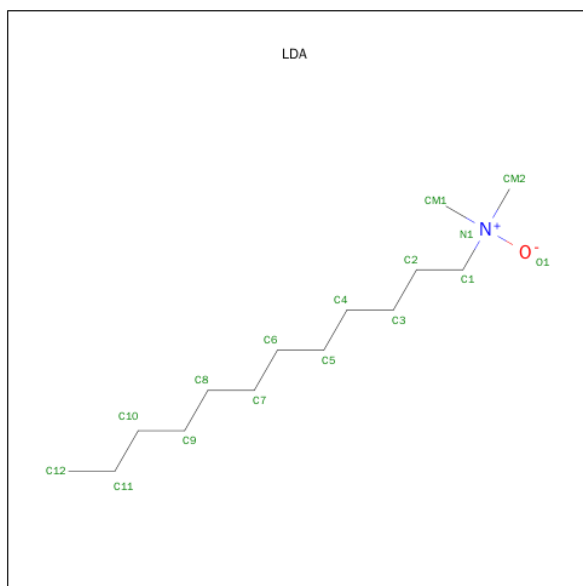
- Molecule 12 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



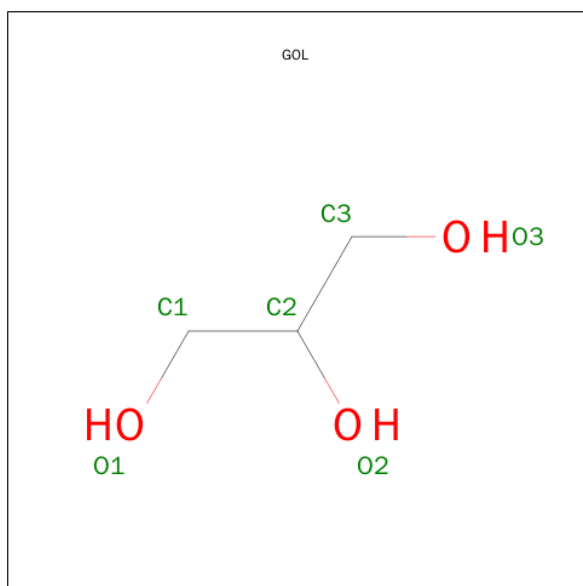
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	L	1	Total	C	N	O	0	0
			16	14	1	1		
13	L	1	Total	C	N	O	0	0
			16	14	1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	L	1	Total	C	O	0	0
			6	3	3		

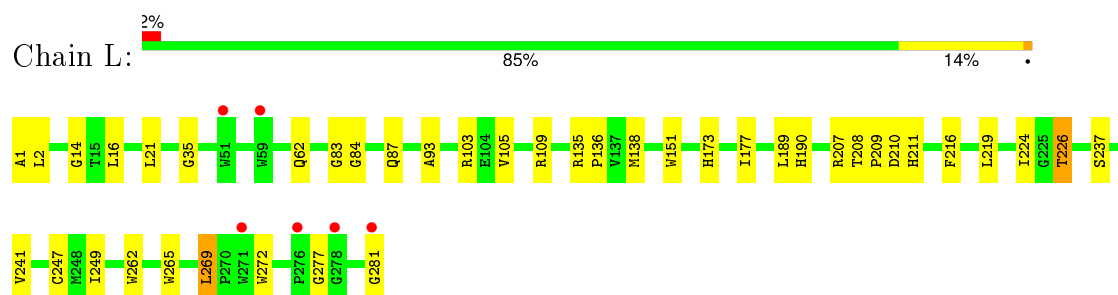
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	147	Total	O	0	0
			147	147		
15	L	109	Total	O	0	0
			109	109		
15	M	108	Total	O	0	0
			108	108		

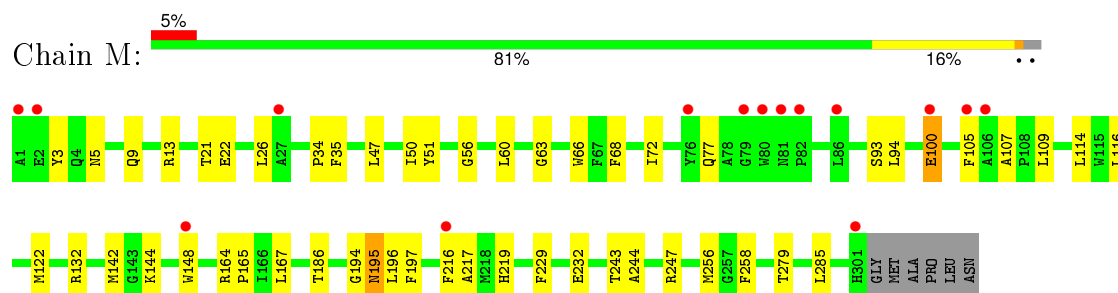
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

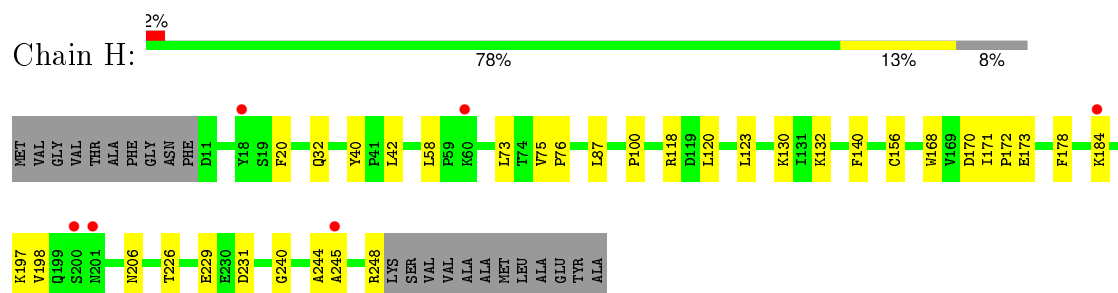
#### • Molecule 1: Reaction center protein L chain



#### • Molecule 2: Reaction center protein M chain



#### • Molecule 3: Reaction center protein H chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.44Å 139.44Å 185.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.34 – 2.25 43.20 – 2.25	Depositor EDS
% Data completeness (in resolution range)	84.8 (39.34-2.25) 84.9 (43.20-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.197 , 0.216 0.187 , 0.206	Depositor DCC
$R_{free}$ test set	4275 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.6	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 84140 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: BCL, GOL, LDA, CL, CDL, BPH, PO4, HTO, FE2, SPO, U10

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	L	0.38	0/2321	0.55	0/3177
2	M	0.38	0/2513	0.52	0/3432
3	H	0.33	0/1862	0.59	0/2534
All	All	0.37	0/6696	0.55	0/9143

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	L	2233	0	2187	34	0
2	M	2418	0	2320	49	0
3	H	1814	0	1818	26	0
4	M	1	0	0	0	0
5	M	1	0	0	1	0
6	M	10	0	0	0	0
7	L	132	0	146	5	0
7	M	198	0	222	11	0
8	L	51	0	45	5	0
9	L	31	0	23	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	15	0	11	2	0
10	M	42	0	60	1	0
11	M	81	0	106	1	0
12	L	10	0	16	0	0
13	L	32	0	62	0	0
13	M	11	0	18	1	0
14	L	6	0	4	0	0
15	H	147	0	0	1	0
15	L	109	0	0	0	0
15	M	108	0	0	0	0
All	All	7450	0	7038	110	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 8.

The worst 5 of 110 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:L:224:ILE:H	9:L:858:U10:H4M3	1.41	0.84
7:L:854:BCL:HMB1	7:L:854:BCL:HBB2	1.63	0.78
2:M:77:GLN:HE22	2:M:93:SER:H	1.32	0.76
2:M:9:GLN:NE2	3:H:198:VAL:H	1.83	0.76
2:M:9:GLN:HE22	3:H:198:VAL:H	1.33	0.73

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
2	M	299/307 (97%)	289 (97%)	10 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	236/260 (91%)	232 (98%)	4 (2%)	0	100	100
All	All	814/848 (96%)	793 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	214 (97%)	6 (3%)	52	63
2	M	238/242 (98%)	234 (98%)	4 (2%)	68	79
3	H	193/208 (93%)	190 (98%)	3 (2%)	70	81
All	All	651/670 (97%)	638 (98%)	13 (2%)	63	73

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	272	TRP
2	M	94	LEU
3	H	73	LEU
1	L	269	LEU
2	M	216	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	9	GLN
3	H	206	ASN
2	M	195	ASN
1	L	211	HIS
2	M	77	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	BCL	L	852	1	53,74,74	1.80	7 (13%)	57,115,115	1.95	14 (24%)
7	BCL	L	854	1	53,74,74	1.86	8 (15%)	57,115,115	2.07	13 (22%)
8	BPH	L	855	-	50,56,70	2.76	18 (36%)	56,84,101	2.77	16 (28%)
9	U10	L	858	-	16,16,63	1.96	4 (25%)	18,22,79	2.20	4 (22%)
9	U10	L	859	-	15,15,63	1.81	4 (26%)	19,21,79	2.16	4 (21%)
12	HTO	L	863	-	9,9,9	0.82	0	8,10,10	1.90	1 (12%)
13	LDA	L	864	-	15,15,15	4.23	1 (6%)	16,17,17	1.72	3 (18%)
13	LDA	L	865	-	15,15,15	4.33	1 (6%)	16,17,17	1.67	1 (6%)
14	GOL	L	869	-	5,5,5	4.88	5 (100%)	5,5,5	5.66	3 (60%)
7	BCL	M	851	2	53,74,74	1.84	9 (16%)	57,115,115	2.24	19 (33%)
7	BCL	M	853	2	53,74,74	1.95	6 (11%)	57,115,115	2.14	19 (33%)
7	BCL	M	856	2	53,74,74	2.00	8 (15%)	57,115,115	1.88	15 (26%)
9	U10	M	857	-	15,15,63	1.98	4 (26%)	19,21,79	2.15	4 (21%)
10	SPO	M	860	-	40,41,41	1.48	7 (17%)	45,50,50	3.91	14 (31%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CDL	M	862	-	80,80,99	1.44	6 (7%)	82,92,111	1.60	14 (17%)
13	LDA	M	866	-	10,10,15	4.59	1 (10%)	11,12,17	2.28	4 (36%)
6	PO4	M	867	-	4,4,4	0.66	0	6,6,6	0.31	0
6	PO4	M	868	-	4,4,4	0.45	0	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	L	852	1	2/2/21/25	0/37/137/137	0/0/9/9
7	BCL	L	854	1	2/2/21/25	0/37/137/137	0/0/9/9
8	BPH	L	855	-	-	0/38/89/105	0/1/6/6
9	U10	L	858	-	-	0/7/31/87	0/1/1/1
9	U10	L	859	-	-	0/6/30/87	0/1/1/1
12	HTO	L	863	-	-	0/10/10/10	0/0/0/0
13	LDA	L	864	-	-	0/13/13/13	0/0/0/0
13	LDA	L	865	-	-	0/13/13/13	0/0/0/0
14	GOL	L	869	-	-	0/4/4/4	0/0/0/0
7	BCL	M	851	2	2/2/21/25	0/37/137/137	0/0/9/9
7	BCL	M	853	2	2/2/21/25	0/37/137/137	0/0/9/9
7	BCL	M	856	2	2/2/21/25	0/37/137/137	0/0/9/9
9	U10	M	857	-	-	0/6/30/87	0/1/1/1
10	SPO	M	860	-	-	0/47/47/47	0/0/0/0
11	CDL	M	862	-	-	0/91/91/110	0/0/0/0
13	LDA	M	866	-	-	0/8/8/13	0/0/0/0
6	PO4	M	867	-	-	0/0/0/0	0/0/0/0
6	PO4	M	868	-	-	0/0/0/0	0/0/0/0

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	865	LDA	O1-N1	-16.49	1.23	1.39
13	L	864	LDA	O1-N1	-15.76	1.24	1.39
13	M	866	LDA	O1-N1	-14.23	1.26	1.39
14	L	869	GOL	C3-C2	-8.50	1.19	1.52
8	L	855	BPH	C3D-C4D	-4.65	1.35	1.41

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	860	SPO	C18-C17-C19	-15.12	100.57	122.90
10	M	860	SPO	C20-C21-C22	-10.05	101.16	123.39
8	L	855	BPH	OBD-CAD-CBD	-7.79	114.18	125.94
7	M	851	BCL	OBD-CAD-CBD	-7.15	115.15	125.94
7	M	853	BCL	CMB-C2B-C1B	-6.84	117.05	128.36

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	M	851	BCL	C8
7	M	851	BCL	C13
7	M	856	BCL	C8
7	M	856	BCL	C13
7	L	854	BCL	C8

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	852	BCL	3	0
7	L	854	BCL	3	0
8	L	855	BPH	5	0
9	L	858	U10	4	0
7	M	851	BCL	2	0
7	M	853	BCL	4	0
7	M	856	BCL	5	0
9	M	857	U10	2	0
10	M	860	SPO	1	0
11	M	862	CDL	1	0
13	M	866	LDA	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	L	281/281 (100%)	-0.39	6 (2%) 67 71	18, 26, 48, 57	0
2	M	301/307 (98%)	-0.12	15 (4%) 32 36	17, 30, 49, 72	0
3	H	238/260 (91%)	-0.37	6 (2%) 61 65	20, 29, 43, 71	0
All	All	820/848 (96%)	-0.28	27 (3%) 50 55	17, 28, 48, 72	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	5.9
3	H	18	TYR	3.3
3	H	60	LYS	3.2
2	M	2	GLU	3.1
1	L	281	GLY	2.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	GOL	L	869	6/6	0.83	0.29	22.61	50,54,56,58	0
13	LDA	L	865	16/16	0.67	0.38	19.29	70,73,78,79	0
13	LDA	L	864	16/16	0.66	0.34	13.00	54,66,74,74	0
12	HTO	L	863	10/10	0.84	0.23	12.18	59,61,62,63	0
11	CDL	M	862	81/100	0.75	0.29	3.20	61,72,89,93	0
13	LDA	M	866	11/16	0.74	0.35	2.61	77,79,83,83	0
9	U10	M	857	15/63	0.80	0.23	1.86	59,63,65,66	0
9	U10	L	858	16/63	0.84	0.19	1.52	34,38,43,45	0
6	PO4	M	867	5/5	0.95	0.22	1.01	67,68,68,69	0
7	BCL	M	851	66/66	0.96	0.13	0.90	17,23,66,68	0
10	SPO	M	860	42/42	0.91	0.14	0.81	27,35,58,61	0
9	U10	L	859	15/63	0.94	0.16	0.74	40,44,48,49	0
7	BCL	M	853	66/66	0.96	0.14	0.56	19,24,44,53	0
7	BCL	L	852	66/66	0.97	0.11	0.31	15,22,43,52	0
7	BCL	M	856	66/66	0.97	0.11	0.13	12,20,32,34	0
5	CL	M	861	1/1	1.00	0.17	0.08	24,24,24,24	0
6	PO4	M	868	5/5	0.97	0.10	0.06	57,58,59,59	0
7	BCL	L	854	66/66	0.96	0.11	-0.21	19,23,50,51	0
8	BPH	L	855	51/65	0.96	0.12	-0.27	22,27,42,46	0
4	FE2	M	850	1/1	1.00	0.12	-1.75	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.