



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:14 am GMT

PDB ID : 1K6L  
Title : Photosynthetic Reaction Center from Rhodobacter sphaeroides  
Authors : Pokkuluri, P.R.; Laible, P.D.; Deng, Y.-L.; Wong, T.N.; Hanson, D.K.; Schiffer, M.  
Deposited on : 2001-10-16  
Resolution : 3.10 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

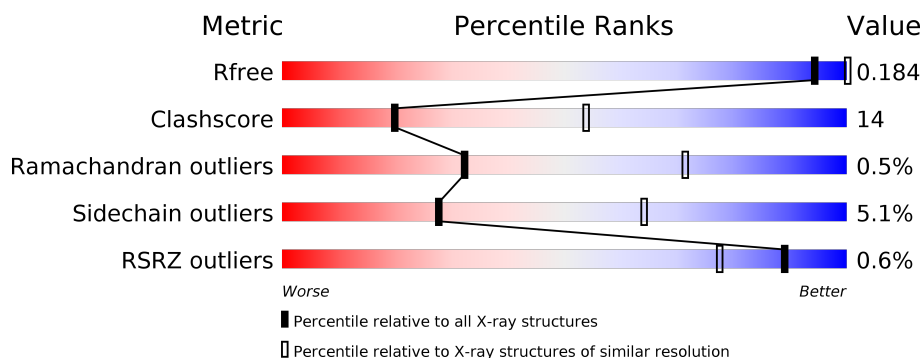
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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>70%</div> <div>26%</div> <div>• •</div> </div>
2	M	314	<div> <div>%</div> <div>66%</div> <div>26%</div> <div>5%</div> <div>•</div> </div>
3	H	260	<div> <div>%</div> <div>62%</div> <div>26%</div> <div>•</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
10	LDA	H	703	-	-	-	X
10	LDA	L	709	-	-	-	X
10	LDA	M	701	-	-	-	X
10	LDA	M	704	-	-	-	X
5	BCL	L	304	X	-	-	-
5	BCL	M	501	X	-	-	X
6	BPH	M	401	X	-	-	-
7	U10	L	502	-	-	-	X
8	SPN	M	600	-	-	-	X
9	CDL	M	800	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7285 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 PHOTOSYNTHETIC REACTION CENTER L SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	308	HIS	-	EXPRESSION TAG	UNP P02953
M	309	HIS	-	EXPRESSION TAG	UNP P02953
M	310	HIS	-	EXPRESSION TAG	UNP P02953
M	311	HIS	-	EXPRESSION TAG	UNP P02953
M	312	HIS	-	EXPRESSION TAG	UNP P02953
M	313	HIS	-	EXPRESSION TAG	UNP P02953
M	314	HIS	-	EXPRESSION TAG	UNP P02953

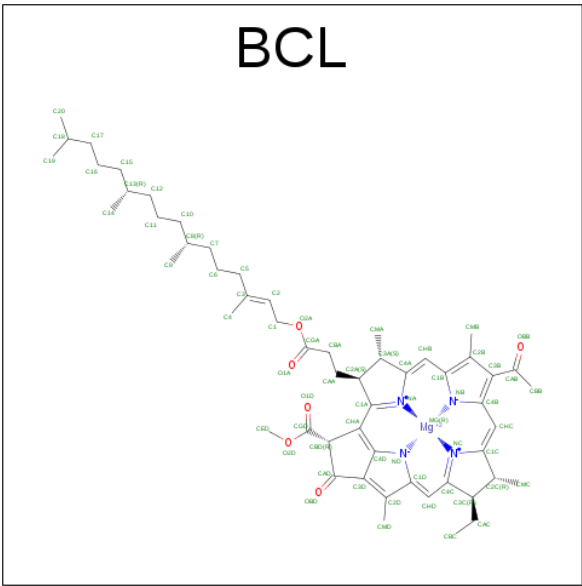
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER H SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

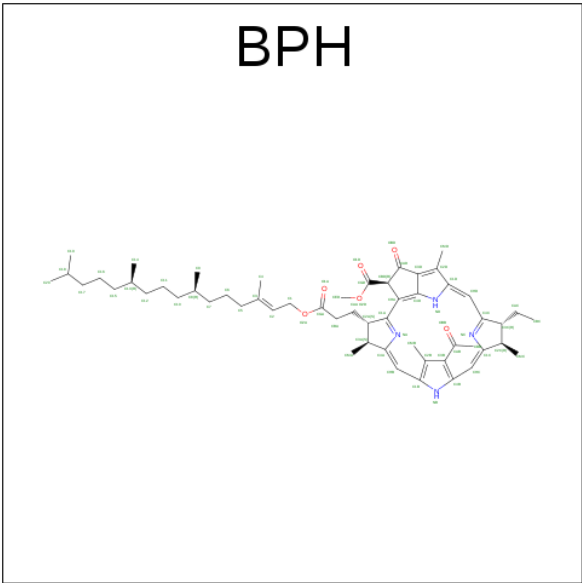
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



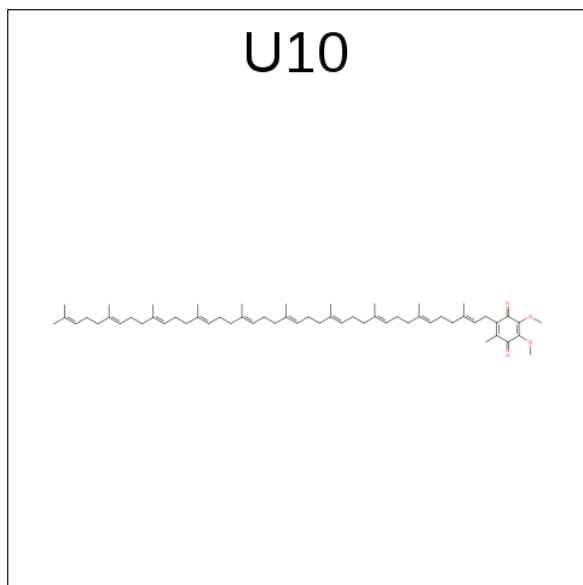
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



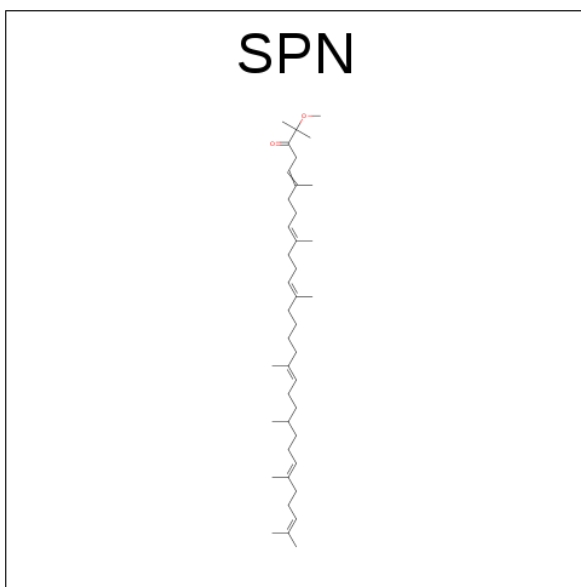
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	10	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



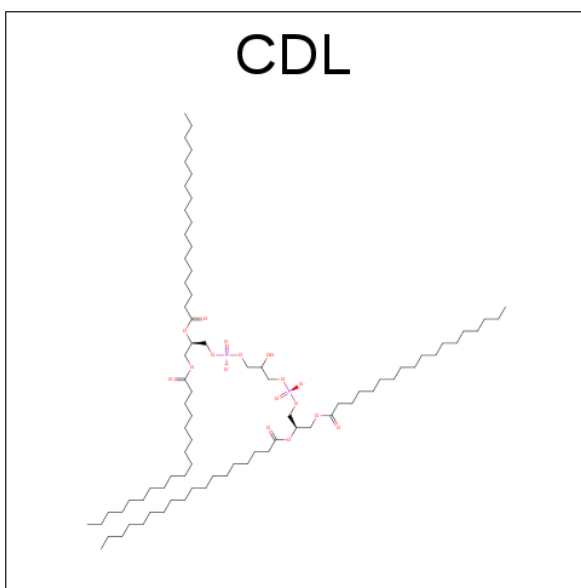
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		
7	L	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is SPEROIDENONE (three-letter code: SPN) (formula:  $C_{41}H_{70}O_2$ ).



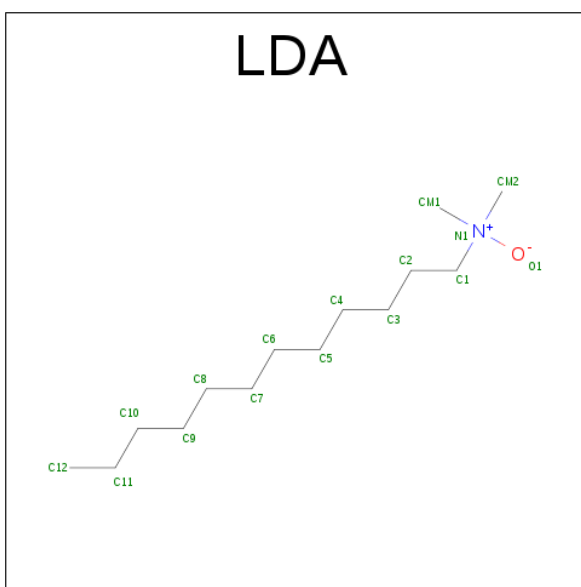
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	H	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	L	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	60	Total	O	0	0
			60	60		
11	L	37	Total	O	0	0
			37	37		
11	M	40	Total	O	0	0
			40	40		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.50Å 141.50Å 187.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.10 19.95 – 3.10	Depositor EDS
% Data completeness (in resolution range)	81.4 (10.00-3.10) 92.2 (19.95-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.90 (at 3.09Å)	Xtriage
Refinement program	?	Depositor
R, $R_{free}$	0.193 , 0.194 0.186 , 0.184	Depositor DCC
$R_{free}$ test set	2565 reflections (7.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.6	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 78.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, CDL, BPH, FE, SPN, 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	0.95	0/2320	1.09	14/3175 (0.4%)
2	M	1.03	0/2500	1.10	16/3413 (0.5%)
3	H	0.92	1/1877 (0.1%)	1.20	19/2553 (0.7%)
All	All	0.97	1/6697 (0.0%)	1.13	49/9141 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	250	SER	C-O	5.51	1.33	1.23

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	103	ARG	NE-CZ-NH1	11.03	125.82	120.30
1	L	217	ARG	NE-CZ-NH2	8.65	124.62	120.30
3	H	202	ARG	NE-CZ-NH2	7.42	124.01	120.30
3	H	154	ARG	NE-CZ-NH2	7.38	123.99	120.30
3	H	117	ARG	NE-CZ-NH2	7.33	123.96	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	280	ASN	Mainchain

## 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	L	2232	0	2187	72	0
2	M	2408	0	2321	76	0
3	H	1829	0	1836	48	0
4	M	1	0	0	0	0
5	L	132	0	148	16	0
5	M	132	0	148	18	0
6	L	65	0	76	2	0
6	M	65	0	76	1	0
7	L	48	0	63	6	0
7	M	48	0	63	6	0
8	M	43	0	69	1	0
9	M	81	0	106	1	0
10	H	16	0	31	4	0
10	L	16	0	31	3	0
10	M	32	0	62	4	0
11	H	60	0	0	2	0
11	L	37	0	0	1	0
11	M	40	0	0	1	0
All	All	7285	0	7217	203	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 14.

The worst 5 of 203 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)
3:H:33:THR:O	3:H:59:PRO:HG3	1.69	0.91
1:L:34:PHE:O	1:L:38:THR:HG23	1.71	0.89
7:M:503:U10:H202	10:H:703:LDA:H112	1.54	0.88
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.56	0.85
2:M:197:PHE:HZ	5:M:502:BCL:HBB2	1.47	0.80

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%)	265 (95%)	14 (5%)	0	100	100
2	M	300/314 (96%)	285 (95%)	11 (4%)	4 (1%)	14	48
3	H	238/260 (92%)	229 (96%)	9 (4%)	0	100	100
All	All	817/855 (96%)	779 (95%)	34 (4%)	4 (0%)	32	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	22	GLU
2	M	301	HIS
2	M	52	LEU
2	M	34	PRO

### 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%)	208 (94%)	12 (6%)	25	61
2	M	236/247 (96%)	226 (96%)	10 (4%)	34	71
3	H	195/208 (94%)	184 (94%)	11 (6%)	25	61
All	All	651/675 (96%)	618 (95%)	33 (5%)	28	64

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	136	ARG
2	M	204	LEU
3	H	225	VAL
2	M	144	LYS
2	M	152	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	280	ASN
2	M	4	GLN
2	M	188	ASN
3	H	206	ASN

### 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 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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
10	LDA	H	703	-	13,15,15	2.84	2 (15%)	14,17,17	0.84	1 (7%)
5	BCL	L	302	1	55,74,74	1.63	8 (14%)	65,115,115	1.90	11 (16%)
5	BCL	L	304	1	55,74,74	1.48	7 (12%)	65,115,115	1.93	11 (16%)
6	BPH	L	402	-	65,70,70	1.29	9 (13%)	75,101,101	1.92	20 (26%)
7	U10	L	502	-	48,48,63	2.08	20 (41%)	58,61,79	0.98	3 (5%)
10	LDA	L	709	-	13,15,15	2.76	1 (7%)	14,17,17	0.69	0
6	BPH	M	401	-	65,70,70	1.30	7 (10%)	75,101,101	2.29	26 (34%)
5	BCL	M	501	2	55,74,74	1.73	9 (16%)	65,115,115	2.38	23 (35%)
5	BCL	M	502	2	55,74,74	1.24	5 (9%)	65,115,115	1.59	11 (16%)
7	U10	M	503	-	48,48,63	2.38	20 (41%)	58,61,79	1.25	7 (12%)
8	SPN	M	600	-	40,42,42	3.61	18 (45%)	48,52,52	2.60	16 (33%)
10	LDA	M	701	-	13,15,15	2.93	1 (7%)	14,17,17	0.49	0
10	LDA	M	704	-	13,15,15	2.33	1 (7%)	14,17,17	0.68	0
9	CDL	M	800	-	80,80,99	0.48	0	82,92,111	0.96	5 (6%)

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
10	LDA	H	703	-	-	0/13/13/13	0/0/0/0
5	BCL	L	302	1	-	0/37/137/137	0/0/9/9
5	BCL	L	304	1	1/1/21/25	0/37/137/137	0/0/9/9
6	BPH	L	402	-	-	0/54/105/105	0/1/6/6
7	U10	L	502	-	-	0/45/69/87	0/1/1/1
10	LDA	L	709	-	-	0/13/13/13	0/0/0/0
6	BPH	M	401	-	1/1/18/22	0/54/105/105	0/1/6/6
5	BCL	M	501	2	2/2/21/25	1/37/137/137	0/0/9/9
5	BCL	M	502	2	-	0/37/137/137	0/0/9/9
7	U10	M	503	-	-	0/45/69/87	0/1/1/1
8	SPN	M	600	-	-	0/50/51/51	0/0/0/0
10	LDA	M	701	-	-	0/13/13/13	0/0/0/0
10	LDA	M	704	-	-	0/13/13/13	0/0/0/0
9	CDL	M	800	-	-	0/91/91/110	0/0/0/0

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	701	LDA	O1-N1	-10.41	1.21	1.42
10	H	703	LDA	O1-N1	-9.90	1.22	1.42
10	L	709	LDA	O1-N1	-9.84	1.22	1.42
10	M	704	LDA	O1-N1	-8.29	1.25	1.42
7	M	503	U10	C27-C28	-7.01	1.26	1.50

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	304	BCL	O1D-CGD-CBD	-6.35	113.20	124.60
5	M	501	BCL	C4-C3-C5	-5.77	105.27	115.29
6	L	402	BPH	O2A-CGA-O1A	-5.18	110.68	123.55
8	M	600	SPN	C6-C5-C4	-5.09	110.68	121.10
8	M	600	SPN	C17-C18-C19	-4.82	111.24	121.10

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	304	BCL	C13
5	M	501	BCL	C8
5	M	501	BCL	C13
6	M	401	BPH	C8

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	501	BCL	C1-C2-C3-C4

There are no ring outliers.

13 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	703	LDA	4	0
5	L	302	BCL	11	0
5	L	304	BCL	7	0
6	L	402	BPH	2	0
7	L	502	U10	6	0
10	L	709	LDA	3	0
6	M	401	BPH	1	0
5	M	501	BCL	8	0
5	M	502	BCL	12	0
7	M	503	U10	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	600	SPN	1	0
10	M	701	LDA	4	0
9	M	800	CDL	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%)	-0.82	1 (0%) 92 84	10, 27, 66, 94	0
2	M	302/314 (96%)	-0.83	2 (0%) 87 75	11, 32, 68, 97	0
3	H	240/260 (92%)	-0.69	2 (0%) 86 71	13, 29, 58, 95	0
All	All	823/855 (96%)	-0.79	5 (0%) 89 77	10, 29, 66, 97	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	4.6
3	H	249	LYS	3.4
2	M	1	ALA	3.0
2	M	302	GLY	2.8
1	L	281	GLY	2.0

### 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
7	U10	L	502	48/63	0.75	0.56	16.01	61,76,89,90	0
10	LDA	L	709	16/16	0.74	0.43	8.84	67,85,95,97	0
10	LDA	M	704	16/16	0.75	0.36	6.36	48,75,109,109	0
10	LDA	H	703	16/16	0.86	0.31	6.17	34,50,64,67	0
8	SPN	M	600	43/43	0.84	0.30	4.13	36,47,64,67	0
9	CDL	M	800	81/100	0.77	0.41	3.08	41,62,76,77	81
10	LDA	M	701	16/16	0.92	0.21	2.96	29,44,52,58	0
5	BCL	M	501	66/66	0.93	0.20	2.72	27,32,92,94	0
7	U10	M	503	48/63	0.93	0.18	1.88	15,29,60,62	0
6	BPH	L	402	65/65	0.96	0.16	1.86	23,27,38,40	0
6	BPH	M	401	65/65	0.97	0.14	0.66	29,33,63,67	10
5	BCL	M	502	66/66	0.97	0.14	0.58	10,19,52,68	0
5	BCL	L	302	66/66	0.98	0.13	0.48	5,17,40,54	0
5	BCL	L	304	66/66	0.97	0.11	-1.00	2,14,40,49	0
4	FE	M	500	1/1	0.99	0.02	-4.40	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.