wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:55 PM GMT

PDB ID	:	4N7K
Title	:	Zinc Substituted Reaction Center of the Rhodobacter sphaeroides
Authors	:	Hardjasa, A.; Murphy, M.E.P.
Deposited on	:	2013-10-15
Resolution	:	2.85 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
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 (1)) were used in the production of this report:

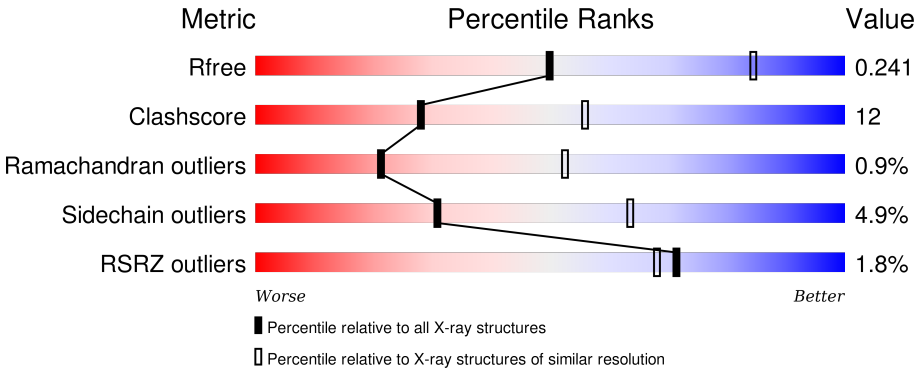
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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.

Mol	Chain	Length	Quality of chain
1	H	241	4% 81% 17%
2	L	281	% 79% 20%
3	M	303	% 76% 22%

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	HTO	L	309	-	-	-	X
10	HTO	L	310	-	-	-	X
13	CDL	M	409	-	-	-	X
14	PC1	M	410	-	-	-	X
4	GOL	H	301	-	-	-	X
4	GOL	L	311	-	-	-	X
4	GOL	L	312	-	-	-	X
5	GGD	H	305	-	-	-	X
7	LDA	L	302	-	-	-	X
7	LDA	L	303	-	-	-	X
7	LDA	L	304	-	-	-	X
7	LDA	M	404	-	-	-	X
8	U10	L	306[A]	-	-	-	X
8	U10	L	306[B]	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7634 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 H Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	241	1849	1183	320	337	9	0	5	1

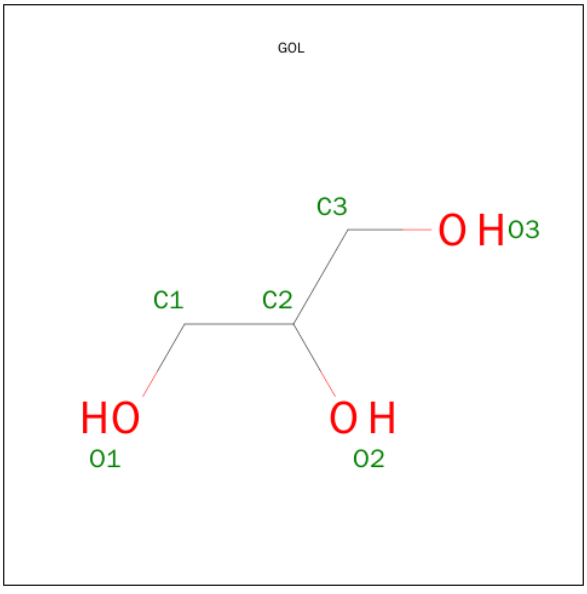
- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2239	1513	355	363	8	0	2	0

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

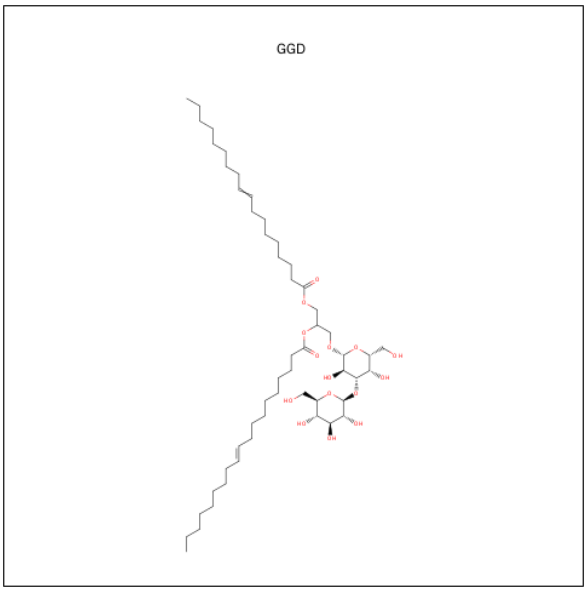
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2411	1607	396	398	10	0	1	1

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



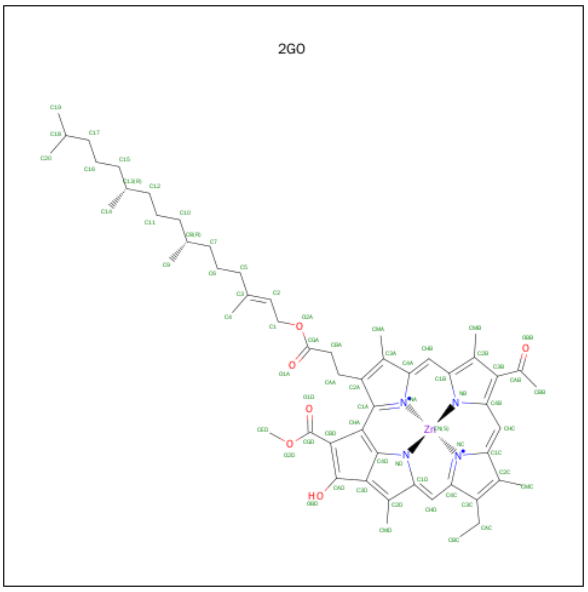
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

- Molecule 5 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-5-(3,4,5-TRIHYDROXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-2-YLOXY)-TETRAHYDRO-PYRAN-2-YLOXY]-1-OCTADEC-9-ENOYLOXYMETHYL-ETHYL ESTER (three-letter code: GGD) (formula: $C_{52}H_{94}O_{15}$).



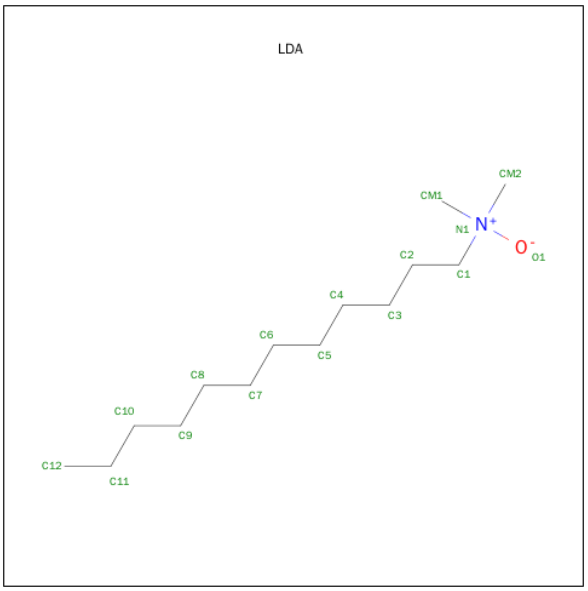
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 57 42 15	0	0

- Molecule 6 is [METHYL 9-ACETYL-14-ETHYL-20-HYDROXY-4,8,13,18-TETRAMETHYL-3-{3-OXO-3-[(3,7,11,15-TETRAMETHYLHEXADEC-2-EN-1-YL)OXY]PROPYL}-3,4,20,21-TETRADEHYDROPHORBINE-21-CARBOXYLATATO(2-)-KAPPA 4 N 23 ,N 24 ,N 25 ,N 26]ZINC (three-letter code: 2GO) (formula: $C_{55}H_{70}N_4O_6Zn$).



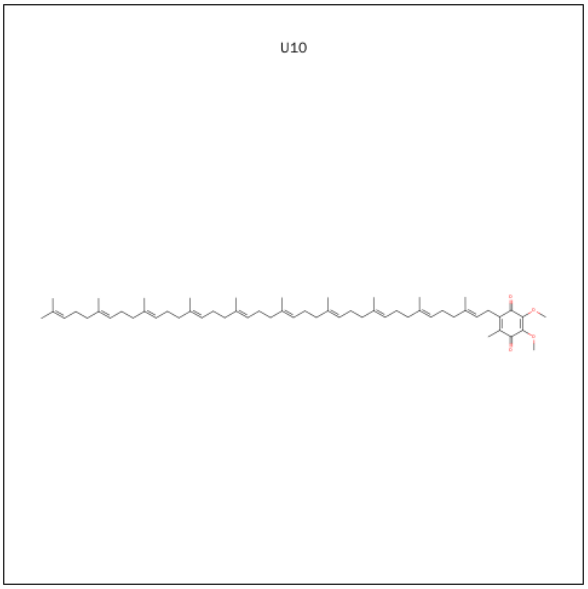
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		
6	L	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		
6	L	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		
6	M	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		
6	M	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		
6	M	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



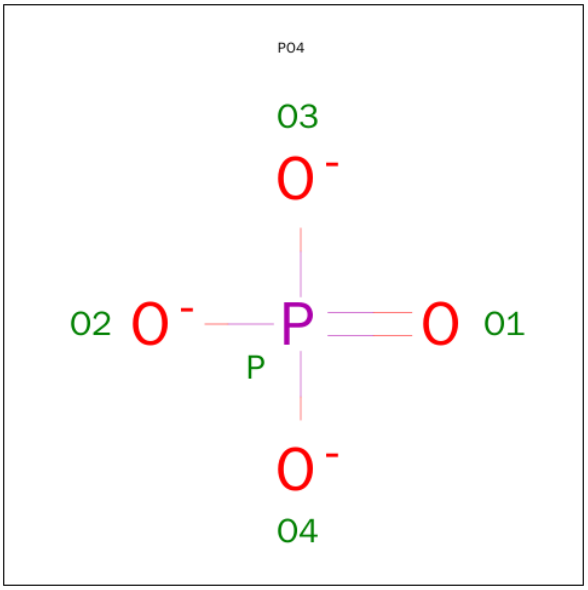
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



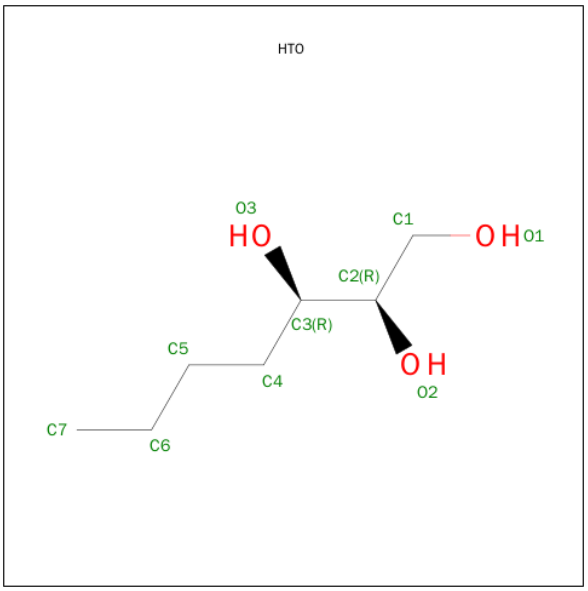
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C O 46 38 8	0	1
8	M	1	Total C O 48 44 4	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total O P 5 4 1	0	0

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

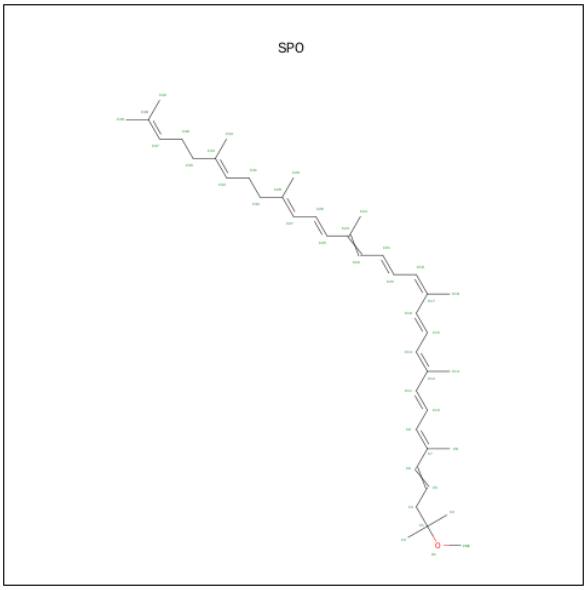


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 10 7 3	0	0
10	L	1	Total C O 10 7 3	0	0

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

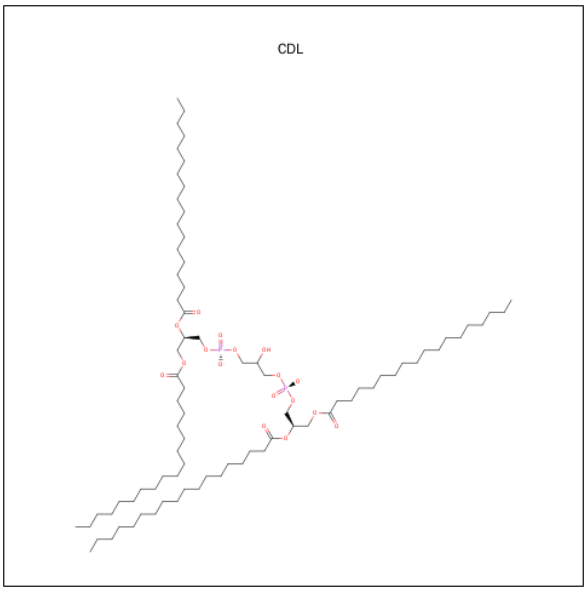
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



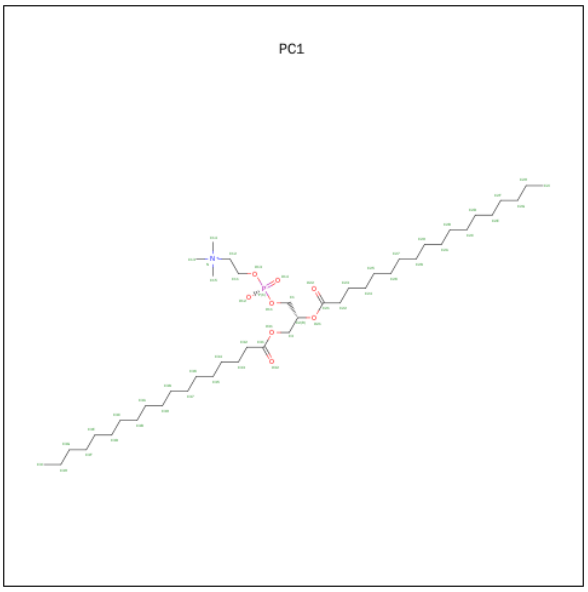
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C O 42 41 1	0	0

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
14	M	1	43	33	1	8	1	0	0

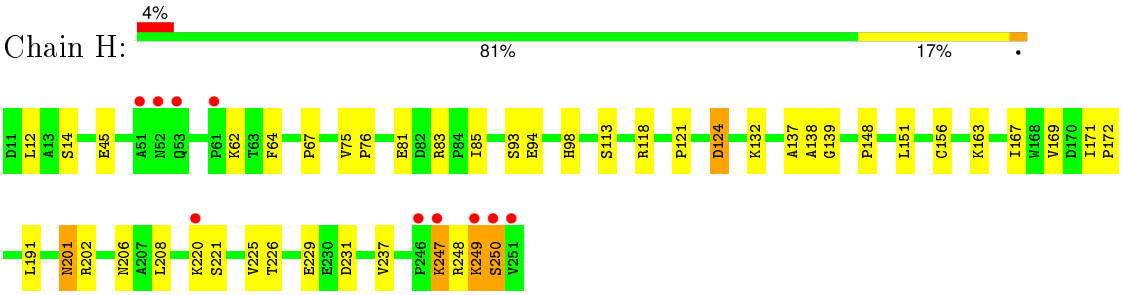
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	109	Total O 109 109	0	0
15	L	81	Total O 81 81	0	0
15	M	84	Total O 84 84	0	0

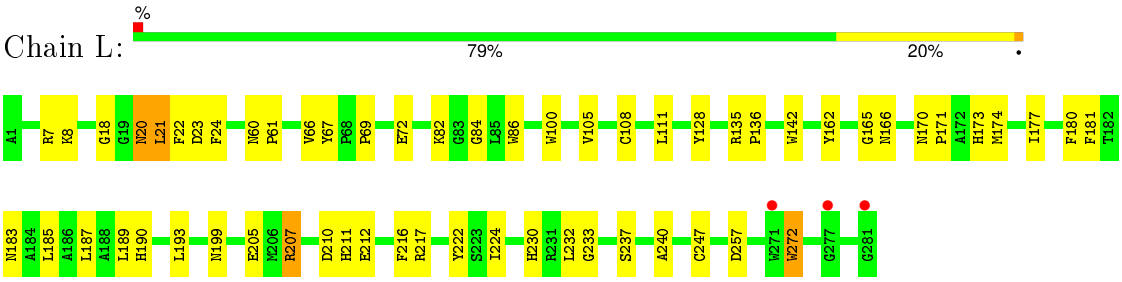
3 Residue-property plots (i)

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.

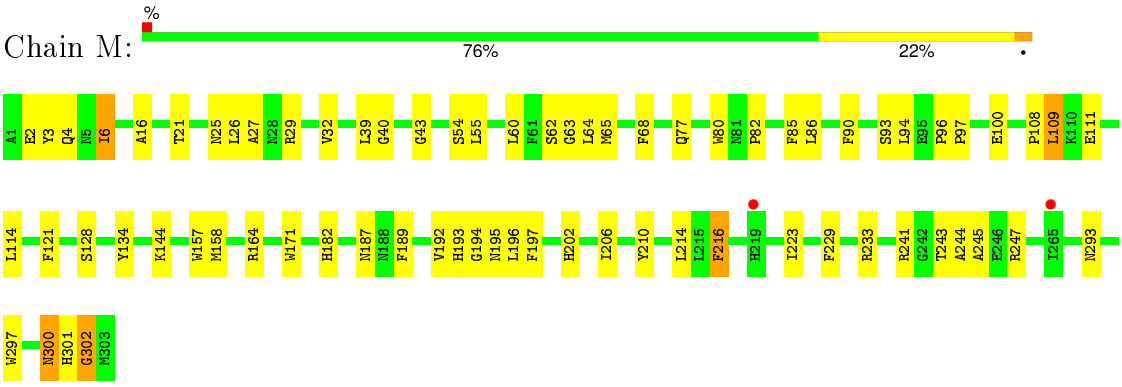
- Molecule 1: Reaction Center H Chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.45Å 139.45Å 184.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.91 – 2.85 36.89 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.0 (36.91-2.85) 96.1 (36.89-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.182 , 0.243 0.182 , 0.241	Depositor DCC
R_{free} test set	2368 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.0	EDS
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 46956 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7634	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, LDA, GGD, CDL, PO4, PC1, HTO, FE, SPO, U10, 2GO

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	H	0.57	0/1929	0.75	0/2619
2	L	0.57	0/2339	0.66	0/3203
3	M	0.58	0/2508	0.69	0/3424
All	All	0.57	0/6776	0.70	0/9246

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	H	1849	0	1872	35	0
2	L	2239	0	2185	61	0
3	M	2411	0	2319	59	0
4	H	24	0	32	3	0
4	L	18	0	24	3	0
5	H	57	0	68	2	0
6	L	198	0	207	14	0
6	M	198	0	207	27	0
7	L	48	0	93	1	0
7	M	32	0	62	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	46	0	46	14	0
8	M	48	0	63	2	0
9	L	5	0	0	1	0
10	L	20	0	32	0	0
11	M	1	0	0	0	0
12	M	42	0	60	5	0
13	M	81	0	106	2	0
14	M	43	0	60	0	0
15	H	109	0	0	6	0
15	L	81	0	0	3	0
15	M	84	0	0	5	0
All	All	7634	0	7436	173	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 12.

The worst 5 of 173 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)
6:L:301:2GO:H9	3:M:206:ILE:HD13	1.48	0.94
3:M:197:PHE:HZ	6:M:402:2GO:H21	1.33	0.93
1:H:118[B]:ARG:HD2	15:M:566:HOH:O	1.72	0.89
3:M:197:PHE:CZ	6:M:402:2GO:H21	2.08	0.88
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.58	0.86

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	H	245/241 (102%)	230 (94%)	11 (4%)	4 (2%)	12 36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	L	281/281 (100%)	262 (93%)	17 (6%)	2 (1%)	26 59
3	M	302/303 (100%)	277 (92%)	23 (8%)	2 (1%)	26 59
All	All	828/825 (100%)	769 (93%)	51 (6%)	8 (1%)	21 49

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	SER
3	M	301	HIS
1	H	249[A]	LYS
1	H	249[B]	LYS
3	M	302	GLY

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	H	199/196 (102%)	184 (92%)	15 (8%)	17 41
2	L	221/220 (100%)	214 (97%)	7 (3%)	46 79
3	M	237/237 (100%)	224 (94%)	13 (6%)	27 58
All	All	657/653 (101%)	622 (95%)	35 (5%)	31 60

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	20	ASN
2	L	210	ASP
3	M	214	LEU
2	L	21	LEU
2	L	72	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	183	ASN
3	M	4	GLN
3	M	187	ASN
2	L	159	ASN
3	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 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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	$\#\|Z\| > 2$
4	GOL	H	301	-	5,5,5	0.37	0	5,5,5	0.51	0
4	GOL	H	302	-	5,5,5	0.74	0	5,5,5	1.05	0
4	GOL	H	303	-	5,5,5	0.46	0	5,5,5	0.43	0
4	GOL	H	304	-	5,5,5	0.39	0	5,5,5	0.56	0
5	GGD	H	305	-	58,58,68	1.01	3 (5%)	72,72,82	1.54	12 (16%)
6	2GO	L	301	2	55,74,74	2.00	12 (21%)	50,115,115	3.16	16 (32%)
7	LDA	L	302	-	15,15,15	3.87	1 (6%)	16,17,17	0.91	1 (6%)
7	LDA	L	303	-	15,15,15	3.85	1 (6%)	16,17,17	0.81	1 (6%)
7	LDA	L	304	-	15,15,15	3.96	1 (6%)	16,17,17	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	2GO	L	305	-	55,74,74	1.88	12 (21%)	50,115,115	3.20	14 (28%)
8	U10	L	306[A]	-	23,23,63	1.72	2 (8%)	28,31,79	1.37	3 (10%)
8	U10	L	306[B]	-	23,23,63	1.60	2 (8%)	28,31,79	1.29	3 (10%)
6	2GO	L	307	2	55,74,74	1.81	12 (21%)	50,115,115	3.34	15 (30%)
9	PO4	L	308	-	4,4,4	0.52	0	6,6,6	0.27	0
10	HTO	L	309	-	9,9,9	0.71	0	8,10,10	0.83	0
10	HTO	L	310	-	9,9,9	0.66	0	8,10,10	0.55	0
4	GOL	L	311	-	5,5,5	0.39	0	5,5,5	0.40	0
4	GOL	L	312	-	5,5,5	0.29	0	5,5,5	0.40	0
4	GOL	L	313	-	5,5,5	0.32	0	5,5,5	0.54	0
6	2GO	M	401	3	55,74,74	1.86	12 (21%)	50,115,115	3.06	14 (28%)
6	2GO	M	402	3	55,74,74	1.86	14 (25%)	50,115,115	3.60	15 (30%)
7	LDA	M	403	-	15,15,15	4.01	1 (6%)	16,17,17	1.10	1 (6%)
7	LDA	M	404	-	15,15,15	3.92	1 (6%)	16,17,17	0.94	1 (6%)
6	2GO	M	406	-	55,74,74	1.84	13 (23%)	50,115,115	3.33	15 (30%)
8	U10	M	407	-	48,48,63	1.35	5 (10%)	58,61,79	1.66	13 (22%)
12	SPO	M	408	-	40,41,41	0.79	0	45,50,50	1.61	11 (24%)
13	CDL	M	409	-	80,80,99	3.46	5 (6%)	82,92,111	1.28	8 (9%)
14	PC1	M	410	-	42,42,53	1.13	2 (4%)	46,50,61	2.55	11 (23%)

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
4	GOL	H	301	-	-	0/4/4/4	0/0/0/0
4	GOL	H	302	-	-	0/4/4/4	0/0/0/0
4	GOL	H	303	-	-	0/4/4/4	0/0/0/0
4	GOL	H	304	-	-	0/4/4/4	0/0/0/0
5	GGD	H	305	-	-	0/47/87/97	0/2/2/2
6	2GO	L	301	2	-	0/37/97/97	0/0/9/9
7	LDA	L	302	-	-	0/13/13/13	0/0/0/0
7	LDA	L	303	-	-	0/13/13/13	0/0/0/0
7	LDA	L	304	-	-	0/13/13/13	0/0/0/0
6	2GO	L	305	-	-	0/37/97/97	0/0/9/9
8	U10	L	306[A]	-	-	0/15/39/87	0/1/1/1
8	U10	L	306[B]	-	-	0/15/39/87	0/1/1/1
6	2GO	L	307	2	-	0/37/97/97	0/0/9/9
9	PO4	L	308	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HTO	L	309	-	-	0/10/10/10	0/0/0/0
10	HTO	L	310	-	-	0/10/10/10	0/0/0/0
4	GOL	L	311	-	-	0/4/4/4	0/0/0/0
4	GOL	L	312	-	-	0/4/4/4	0/0/0/0
4	GOL	L	313	-	-	0/4/4/4	0/0/0/0
6	2GO	M	401	3	-	0/37/97/97	0/0/9/9
6	2GO	M	402	3	-	0/37/97/97	0/0/9/9
7	LDA	M	403	-	-	0/13/13/13	0/0/0/0
7	LDA	M	404	-	-	0/13/13/13	0/0/0/0
6	2GO	M	406	-	-	0/37/97/97	0/0/9/9
8	U10	M	407	-	-	0/45/69/87	0/1/1/1
12	SPO	M	408	-	-	0/47/47/47	0/0/0/0
13	CDL	M	409	-	-	0/91/91/110	0/0/0/0
14	PC1	M	410	-	-	0/46/46/57	0/0/0/0

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	403	LDA	O1-N1	-15.25	1.25	1.39
7	L	304	LDA	O1-N1	-15.19	1.25	1.39
7	M	404	LDA	O1-N1	-14.98	1.25	1.39
7	L	302	LDA	O1-N1	-14.83	1.25	1.39
7	L	303	LDA	O1-N1	-14.74	1.25	1.39

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	307	2GO	CAA-C2A-C1A	-12.65	111.54	127.64
6	L	307	2GO	CAC-C3C-C4C	-11.48	108.68	127.18
6	L	305	2GO	CAA-C2A-C1A	-11.41	113.12	127.64
6	M	402	2GO	CAA-C2A-C1A	-11.07	113.56	127.64
6	L	301	2GO	CAA-C2A-C1A	-10.99	113.66	127.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	301	GOL	2	0
4	H	303	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	305	GGD	2	0
6	L	301	2GO	5	0
7	L	304	LDA	1	0
6	L	305	2GO	8	0
8	L	306[A]	U10	7	0
8	L	306[B]	U10	7	0
6	L	307	2GO	2	0
9	L	308	PO4	1	0
4	L	311	GOL	1	0
4	L	312	GOL	1	0
4	L	313	GOL	1	0
6	M	401	2GO	9	0
6	M	402	2GO	10	0
7	M	403	LDA	1	0
6	M	406	2GO	9	0
8	M	407	U10	2	0
12	M	408	SPO	5	0
13	M	409	CDL	2	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

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^{th} 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^2)	Q<0.9
1	H	241/241 (100%)	-0.33	10 (4%) 41 34	41, 54, 77, 161	3 (1%)
2	L	281/281 (100%)	-0.56	3 (1%) 82 80	37, 53, 79, 101	0
3	M	303/303 (100%)	-0.23	2 (0%) 89 88	37, 55, 81, 123	6 (1%)
All	All	825/825 (100%)	-0.37	15 (1%) 71 68	37, 54, 80, 161	9 (1%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	5.3
1	H	249[A]	LYS	3.8
2	L	281	GLY	3.5
1	H	220[A]	LYS	3.1
1	H	251	VAL	3.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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^{th} 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^2)	Q<0.9
10	HTO	L	310	10/10	0.75	0.82	27.70	86,114,140,156	0
10	HTO	L	309	10/10	0.64	0.87	24.11	88,103,117,127	0
7	LDA	L	302	16/16	0.80	0.40	12.83	42,105,140,143	0
7	LDA	L	303	16/16	0.44	0.56	11.41	76,95,143,148	0
14	PC1	M	410	43/54	0.39	0.49	6.70	78,117,175,190	0
7	LDA	L	304	16/16	0.57	0.39	5.98	68,96,124,125	0
4	GOL	H	301	6/6	0.85	0.43	4.72	94,109,111,112	0
4	GOL	L	312	6/6	0.73	0.35	4.70	87,88,92,95	0
5	GGD	H	305	57/67	0.62	0.54	4.15	49,107,216,221	0
13	CDL	M	409	81/100	0.83	0.37	4.03	70,101,156,164	0
7	LDA	M	404	16/16	0.87	0.39	3.73	67,87,102,106	0
8	U10	L	306[B]	23/63	0.85	0.29	2.64	43,68,73,75	23
4	GOL	L	311	6/6	0.90	0.36	2.57	60,73,85,104	0
8	U10	L	306[A]	23/63	0.85	0.29	2.43	50,71,86,91	23
12	SPO	M	408	42/42	0.94	0.23	1.66	46,64,98,112	0
7	LDA	M	403	16/16	0.94	0.22	1.13	42,60,67,68	0
8	U10	M	407	48/63	0.92	0.31	1.04	43,54,99,111	0
6	2GO	M	401	66/66	0.98	0.18	1.02	35,47,88,92	0
6	2GO	L	307	66/66	0.97	0.15	0.80	35,48,59,63	0
6	2GO	M	406	66/66	0.94	0.20	0.78	60,76,135,142	0
6	2GO	M	402	66/66	0.99	0.17	0.48	39,50,75,86	0
9	PO4	L	308	5/5	0.94	0.13	-0.02	97,97,98,98	0
6	2GO	L	305	66/66	0.98	0.15	-0.03	31,47,56,58	0
6	2GO	L	301	66/66	0.98	0.14	-0.37	29,39,59,68	0
11	FE	M	405	1/1	1.00	0.16	-1.61	46,46,46,46	0
4	GOL	H	302	6/6	0.89	0.45	-	56,65,69,81	0
4	GOL	L	313	6/6	0.89	0.14	-	84,89,93,93	0
4	GOL	H	303	6/6	0.71	0.31	-	73,85,90,96	0
4	GOL	H	304	6/6	0.81	0.24	-	74,85,89,94	0

6.5 Other polymers (i)

There are no such residues in this entry.