wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:06 PM GMT

PDB ID	:	1S00
Title	:	PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-SEPARATED D+QAQB- STATE
Authors	:	Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on	:	2003-12-29
Resolution	:	2.60 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:

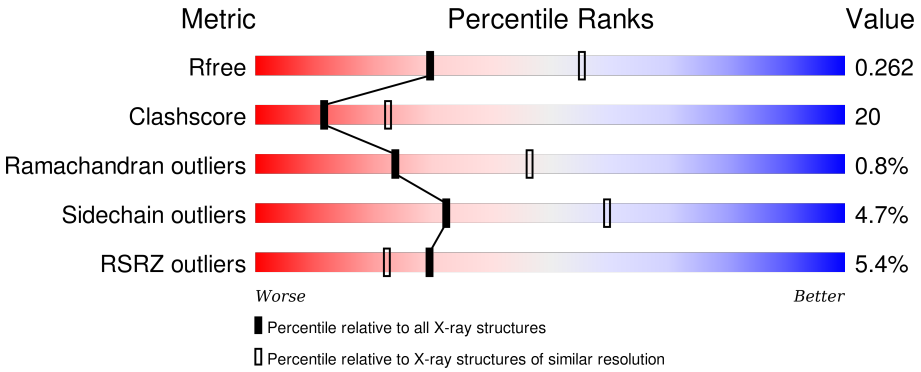
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	L	281	63% 34%
1	R	281	9% 55% 42%
2	M	307	4% 71% 23%
2	S	307	4% 62% 32%
3	H	260	3% 65% 28% 5%

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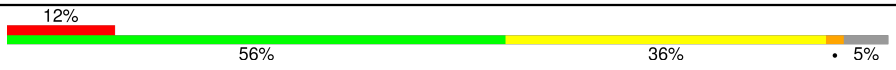
Mol	Chain	Length	Quality of chain
3	T	260	

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
4	BCL	S	2001	-	-	-	X
4	BCL	S	2003	-	-	-	X
5	BPH	L	1006	X	-	-	-
5	BPH	M	1005	X	-	-	-
5	BPH	R	2006	X	-	-	-
6	U10	L	1009[A]	-	-	-	X
6	U10	L	1009[B]	-	-	-	X
6	U10	M	1008	-	-	-	X
6	U10	R	2009[A]	-	-	-	X
6	U10	R	2009[B]	-	-	-	X
8	SPO	M	1010	-	-	-	X
8	SPO	S	2010	-	-	-	X
9	LDA	M	1011	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14144 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
			2232	1507	356	361	8			
1	R	281	Total	C	N	O	S	0	0	0
			2232	1507	356	361	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	213	ASN	ASP	ENGINEERED	UNP P02954
R	213	ASN	ASP	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
			2399	1602	390	396	11			
2	S	299	Total	C	N	O	S	0	0	0
			2385	1594	388	392	11			

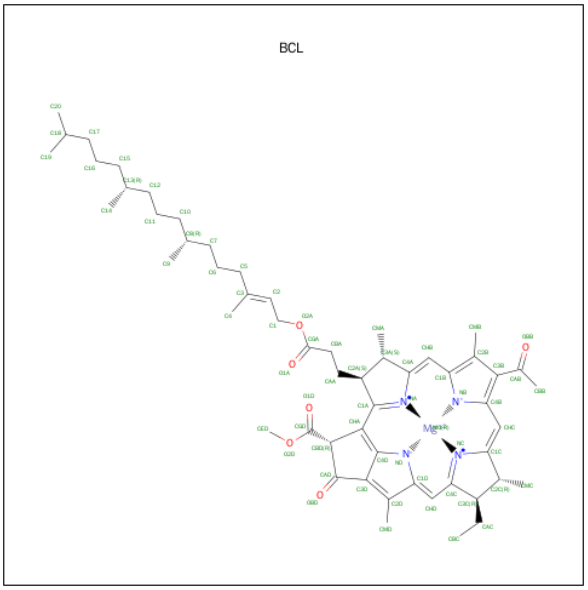
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	233	CYS	ARG	ENGINEERED	UNP P02953
S	233	CYS	ARG	ENGINEERED	UNP P02953

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

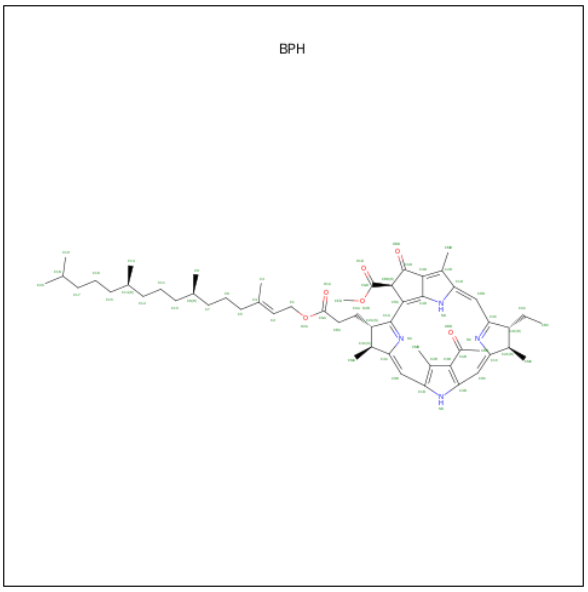
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			
3	T	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



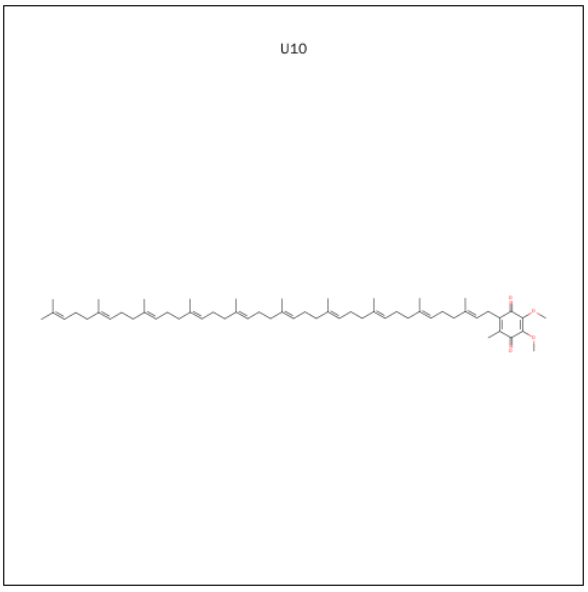
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			55	45	4	6		
5	R	1	Total	C	N	O	0	0
			65	55	4	6		
5	S	1	Total	C	N	O	0	0
			51	41	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

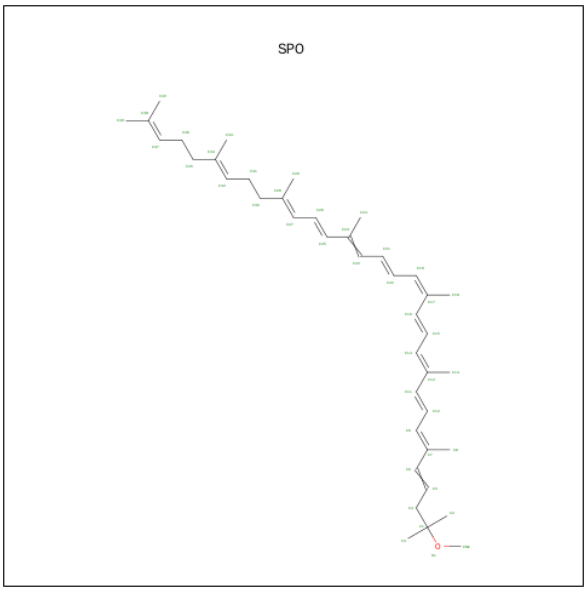


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 60 52 8	0	1
6	M	1	Total C O 38 34 4	0	0
6	R	1	Total C O 36 28 8	0	1
6	S	1	Total C O 32 28 4	0	0

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

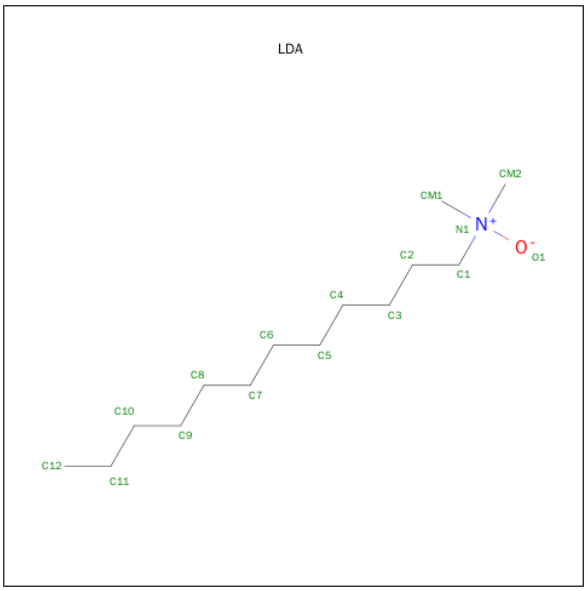
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	S	1	Total Fe 1 1	0	0
7	M	1	Total Fe 1 1	0	0

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

- Molecule 10 is water.

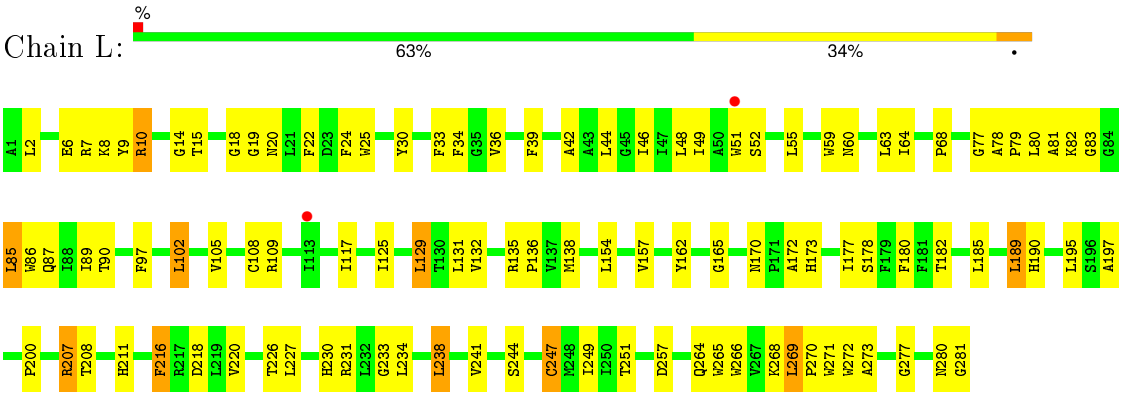
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	26	Total O 26 26	0	0
10	M	42	Total O 42 42	0	0
10	H	39	Total O 39 39	0	0
10	R	13	Total O 13 13	0	0
10	S	24	Total O 24 24	0	0
10	T	12	Total O 12 12	0	0

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.

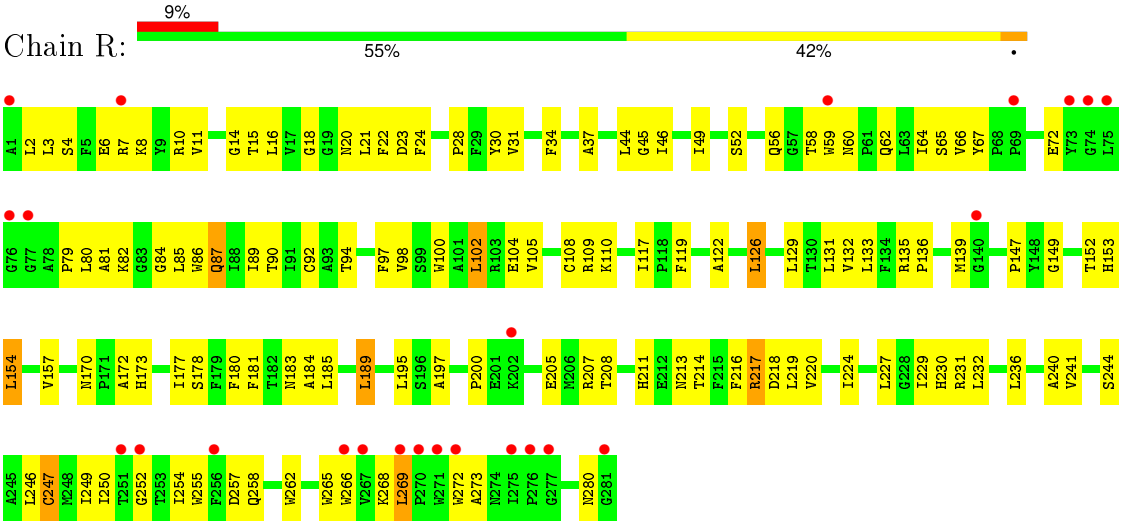
• Molecule 1: Reaction center protein L chain

Chain L:



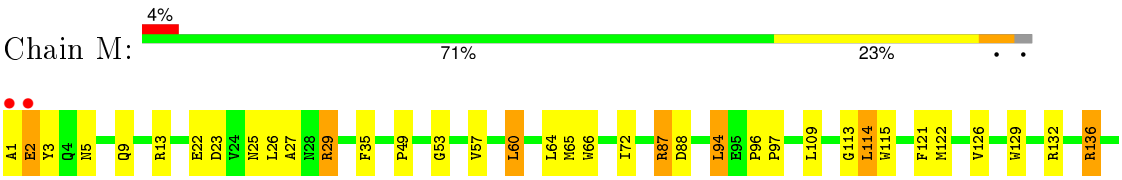
• Molecule 1: Reaction center protein L chain

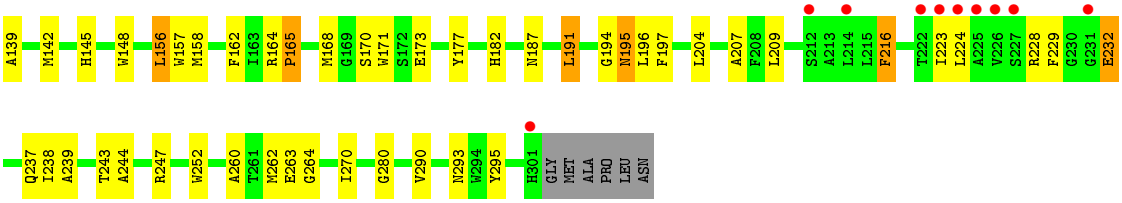
Chain R:



• Molecule 2: Reaction center protein M chain

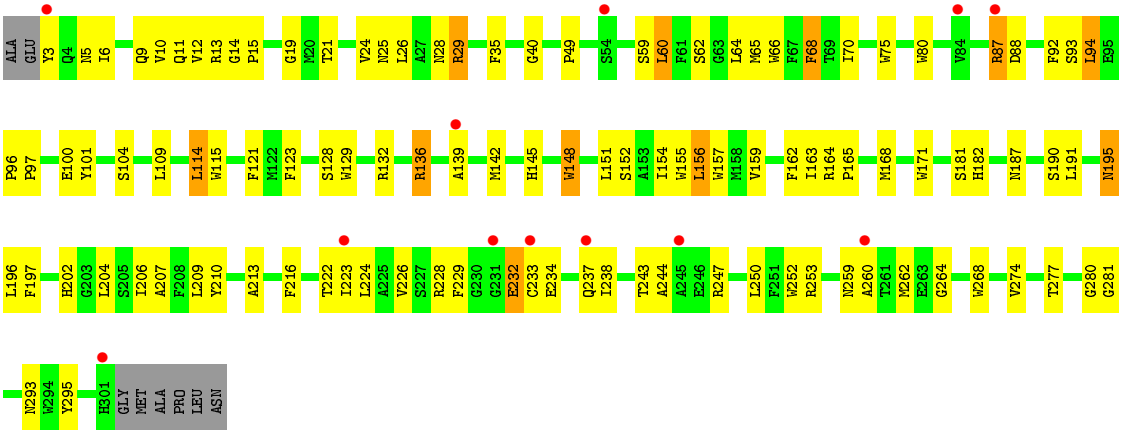
Chain M:





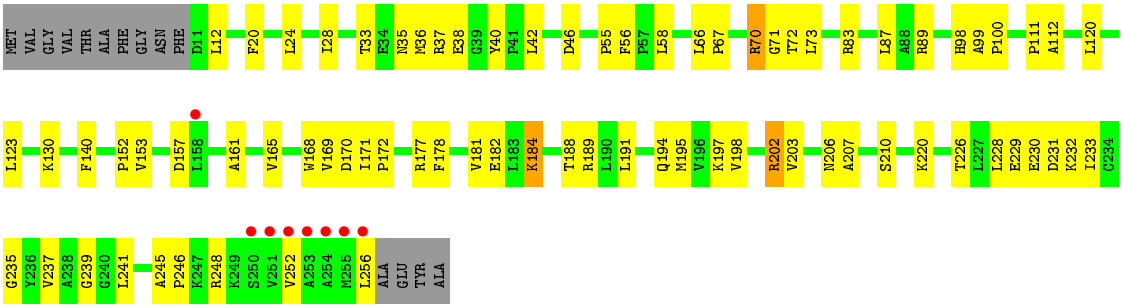
- Molecule 2: Reaction center protein M chain

Chain S:



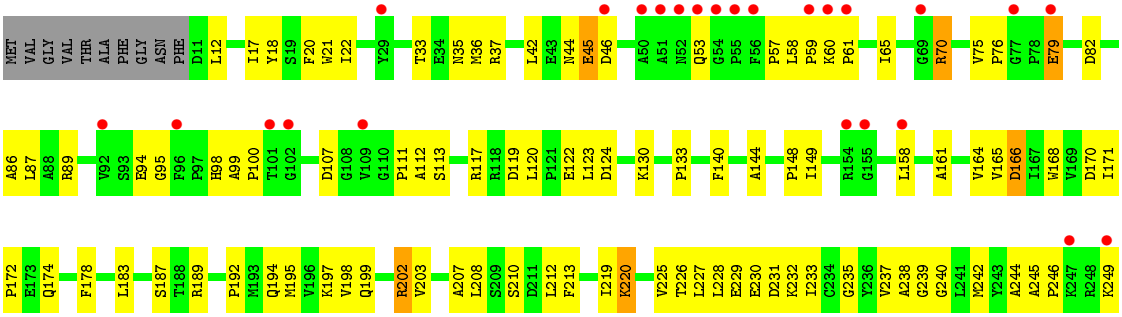
- Molecule 3: Reaction center protein H chain

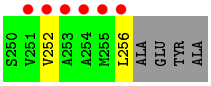
Chain H:



- Molecule 3: Reaction center protein H chain

Chain T:




S250
V251
V252
A253
A254
M255
L256
ALA
GLU
TYR
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	137.73Å 137.73Å 277.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.84 – 2.60 39.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.84-2.60) 94.9 (39.84-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.268 0.223 , 0.262	Depositor DCC
R_{free} test set	3965 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 78308 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14144	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: BCL, LDA, BPH, 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	0.43	0/2320	0.60	0/3175
1	R	0.38	0/2320	0.58	0/3175
2	M	0.42	0/2491	0.59	0/3402
2	S	0.39	0/2477	0.55	0/3383
3	H	0.39	0/1917	0.64	0/2608
3	T	0.33	0/1917	0.60	0/2608
All	All	0.39	0/13442	0.59	0/18351

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	L	2232	0	2189	103	0
1	R	2232	0	2189	120	0
2	M	2399	0	2310	83	0
2	S	2385	0	2296	114	0
3	H	1869	0	1884	74	0
3	T	1869	0	1884	99	0
4	L	183	0	189	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	66	0	74	19	0
4	R	66	0	74	11	0
4	S	183	0	189	29	0
5	L	65	0	74	5	0
5	M	55	0	53	0	0
5	R	65	0	74	8	0
5	S	51	0	45	7	0
6	L	60	0	70	3	0
6	M	38	0	47	0	0
6	R	36	0	30	3	0
6	S	32	0	39	0	0
7	M	1	0	0	0	0
7	S	1	0	0	0	0
8	M	42	0	60	6	0
8	S	42	0	60	2	0
9	M	16	0	31	2	0
10	H	39	0	0	2	0
10	L	26	0	0	4	0
10	M	42	0	0	1	0
10	R	13	0	0	0	0
10	S	24	0	0	2	0
10	T	12	0	0	1	0
All	All	14144	0	13861	565	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 20.

The worst 5 of 565 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:R:200:PRO:HB3	1:R:207:ARG:HD3	1.42	1.02
2:S:157:TRP:HB2	4:S:2003:BCL:H62	1.44	0.99
1:R:219:LEU:HD13	1:R:220:VAL:HG23	1.48	0.95
3:T:226:THR:OG1	3:T:229:GLU:HG3	1.68	0.93
1:R:208:THR:H	1:R:211:HIS:HD2	1.18	0.92

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%)	262 (94%)	16 (6%)	1 (0%)	39 65
1	R	279/281 (99%)	264 (95%)	12 (4%)	3 (1%)	17 36
2	M	299/307 (97%)	280 (94%)	18 (6%)	1 (0%)	46 72
2	S	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	26 51
3	H	244/260 (94%)	233 (96%)	11 (4%)	0	100 100
3	T	244/260 (94%)	223 (91%)	15 (6%)	6 (2%)	7 12
All	All	1642/1696 (97%)	1546 (94%)	83 (5%)	13 (1%)	24 46

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	2	GLU
3	T	45	GLU
3	T	220	LYS
1	R	80	LEU
1	R	257	ASP

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%)	27 51
1	R	220/220 (100%)	210 (96%)	10 (4%)	34 62
2	M	236/240 (98%)	223 (94%)	13 (6%)	27 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	S	235/240 (98%)	221 (94%)	14 (6%)	24 47
3	H	199/208 (96%)	191 (96%)	8 (4%)	38 67
3	T	199/208 (96%)	195 (98%)	4 (2%)	63 85
All	All	1309/1336 (98%)	1248 (95%)	61 (5%)	32 59

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	83	ARG
1	R	102	LEU
2	S	232	GLU
3	H	123	LEU
3	H	191	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	211	HIS
1	R	274	ASN
3	T	53	GLN
3	H	206	ASN
1	R	87	GLN

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 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	BCL	L	1001	-	38,59,74	1.35	4 (10%)	40,97,115	2.13	14 (35%)
4	BCL	L	1002	-	53,74,74	1.04	3 (5%)	57,115,115	1.88	17 (29%)
4	BCL	L	1004	-	53,74,74	1.15	4 (7%)	57,115,115	1.68	15 (26%)
5	BPH	L	1006	-	64,70,70	1.48	8 (12%)	73,101,101	2.18	16 (21%)
6	U10	L	1009[A]	-	30,30,63	2.14	11 (36%)	36,39,79	2.09	13 (36%)
6	U10	L	1009[B]	-	30,30,63	2.05	9 (30%)	36,39,79	2.04	11 (30%)
4	BCL	M	1003	-	53,74,74	1.01	3 (5%)	57,115,115	1.96	21 (36%)
5	BPH	M	1005	-	54,60,70	1.36	7 (12%)	61,89,101	2.32	16 (26%)
6	U10	M	1008	-	38,38,63	2.08	11 (28%)	46,49,79	1.79	9 (19%)
8	SPO	M	1010	-	40,41,41	3.29	22 (55%)	45,50,50	2.54	14 (31%)
9	LDA	M	1011	-	15,15,15	3.66	2 (13%)	16,17,17	2.68	4 (25%)
4	BCL	R	2002	-	53,74,74	1.06	2 (3%)	57,115,115	1.87	18 (31%)
5	BPH	R	2006	-	64,70,70	1.44	8 (12%)	73,101,101	2.20	18 (24%)
6	U10	R	2009[A]	-	18,18,63	2.00	6 (33%)	22,25,79	2.09	5 (22%)
6	U10	R	2009[B]	-	18,18,63	1.98	6 (33%)	22,25,79	2.05	4 (18%)
4	BCL	S	2001	-	38,59,74	1.33	6 (15%)	40,97,115	2.01	14 (35%)
4	BCL	S	2003	-	53,74,74	1.02	1 (1%)	57,115,115	1.95	20 (35%)
4	BCL	S	2004	-	53,74,74	1.12	4 (7%)	57,115,115	1.82	15 (26%)
5	BPH	S	2005	-	50,56,70	1.49	9 (18%)	56,84,101	2.37	15 (26%)
6	U10	S	2008	-	32,32,63	1.98	10 (31%)	38,41,79	1.91	9 (23%)
8	SPO	S	2010	-	40,41,41	3.31	24 (60%)	45,50,50	2.58	12 (26%)

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	BCL	L	1001	-	-	0/19/119/137	0/0/9/9
4	BCL	L	1002	-	-	0/37/137/137	0/0/9/9
4	BCL	L	1004	-	-	0/37/137/137	0/0/9/9
5	BPH	L	1006	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	L	1009[A]	-	-	0/24/48/87	0/1/1/1
6	U10	L	1009[B]	-	-	0/24/48/87	0/1/1/1
4	BCL	M	1003	-	-	0/37/137/137	0/0/9/9
5	BPH	M	1005	-	1/1/16/22	0/42/93/105	0/1/6/6
6	U10	M	1008	-	-	0/33/57/87	0/1/1/1
8	SPO	M	1010	-	-	0/47/47/47	0/0/0/0
9	LDA	M	1011	-	-	0/13/13/13	0/0/0/0
4	BCL	R	2002	-	-	0/37/137/137	0/0/9/9
5	BPH	R	2006	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	R	2009[A]	-	-	0/9/33/87	0/1/1/1
6	U10	R	2009[B]	-	-	0/9/33/87	0/1/1/1
4	BCL	S	2001	-	-	0/19/119/137	0/0/9/9
4	BCL	S	2003	-	-	0/37/137/137	0/0/9/9
4	BCL	S	2004	-	-	0/37/137/137	0/0/9/9
5	BPH	S	2005	-	-	0/38/89/105	0/1/6/6
6	U10	S	2008	-	-	0/26/50/87	0/1/1/1
8	SPO	S	2010	-	-	0/47/47/47	0/0/0/0

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1011	LDA	O1-N1	-13.39	1.26	1.39
5	L	1006	BPH	C11-C10	-5.08	1.28	1.52
5	R	2006	BPH	C11-C10	-5.00	1.29	1.52
4	L	1001	BCL	C3C-C4C	-4.22	1.46	1.51
6	M	1008	U10	C7-C8	-3.84	1.44	1.50

The worst 5 of 280 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	1011	LDA	CM2-N1-CM1	-8.11	99.68	108.83
8	M	1010	SPO	O1-C1-C4	-7.97	86.37	105.87
8	S	2010	SPO	O1-C1-C4	-7.85	86.66	105.87
8	S	2010	SPO	C15-C14-C12	-6.38	117.98	127.20
8	S	2010	SPO	C20-C21-C22	-5.79	110.59	123.39

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1006	BPH	C8
5	L	1006	BPH	C13
5	R	2006	BPH	C8
5	R	2006	BPH	C13
5	M	1005	BPH	C8

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1001	BCL	11	0
4	L	1002	BCL	11	0
4	L	1004	BCL	10	0
5	L	1006	BPH	5	0
6	L	1009[A]	U10	1	0
6	L	1009[B]	U10	2	0
4	M	1003	BCL	19	0
8	M	1010	SPO	6	0
9	M	1011	LDA	2	0
4	R	2002	BCL	11	0
5	R	2006	BPH	8	0
6	R	2009[A]	U10	1	0
6	R	2009[B]	U10	2	0
4	S	2001	BCL	8	0
4	S	2003	BCL	16	0
4	S	2004	BCL	8	0
5	S	2005	BPH	7	0
8	S	2010	SPO	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	L	281/281 (100%)	0.17	2 (0%) 89 87	23, 42, 61, 77	0
1	R	281/281 (100%)	0.46	24 (8%) 13 9	35, 56, 73, 82	0
2	M	301/307 (98%)	0.14	12 (3%) 42 34	26, 38, 53, 85	0
2	S	299/307 (97%)	0.18	12 (4%) 42 34	37, 50, 59, 89	0
3	H	246/260 (94%)	0.06	8 (3%) 50 43	28, 44, 65, 97	0
3	T	246/260 (94%)	0.54	31 (12%) 5 3	47, 62, 84, 99	0
All	All	1654/1696 (97%)	0.26	89 (5%) 29 22	23, 49, 74, 99	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	1	ALA	6.1
3	T	55	PRO	5.7
3	H	252	VAL	5.0
3	T	252	VAL	4.5
3	T	158	LEU	4.2

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 (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^{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
6	U10	L	1009[B]	30/63	0.67	0.64	9.67	44,54,65,66	30
6	U10	R	2009[B]	18/63	0.65	0.53	8.87	95,96,97,97	18
6	U10	L	1009[A]	30/63	0.67	0.64	8.09	54,67,69,70	30
6	U10	R	2009[A]	18/63	0.65	0.53	7.63	94,96,97,98	18
9	LDA	M	1011	16/16	0.74	0.34	7.30	49,61,78,78	0
8	SPO	S	2010	42/42	0.90	0.24	2.37	38,49,64,66	0
4	BCL	S	2001	51/66	0.90	0.23	2.32	38,45,58,61	0
6	U10	M	1008	38/63	0.91	0.36	2.25	36,42,63,64	0
8	SPO	M	1010	42/42	0.90	0.24	2.24	31,36,59,61	0
4	BCL	S	2003	66/66	0.92	0.23	2.01	44,49,62,71	0
6	U10	S	2008	32/63	0.96	0.38	1.97	56,58,64,66	0
5	BPH	L	1006	65/65	0.92	0.29	1.79	24,35,41,43	0
4	BCL	L	1002	66/66	0.90	0.24	1.78	31,36,44,52	0
4	BCL	L	1004	66/66	0.93	0.32	1.76	28,34,57,59	0
4	BCL	S	2004	66/66	0.91	0.23	1.74	44,52,74,75	0
5	BPH	R	2006	65/65	0.90	0.24	1.69	47,56,61,62	0
4	BCL	R	2002	66/66	0.89	0.21	1.30	42,53,56,56	0
4	BCL	L	1001	51/66	0.93	0.23	1.21	26,32,45,48	0
4	BCL	M	1003	66/66	0.93	0.22	1.09	24,38,47,49	0
5	BPH	S	2005	51/65	0.94	0.20	0.85	35,42,51,52	0
5	BPH	M	1005	55/65	0.94	0.21	0.65	26,32,43,46	0
7	FE2	S	2007	1/1	0.98	0.14	-1.79	51,51,51,51	0
7	FE2	M	1007	1/1	0.99	0.15	-2.22	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.