



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:32 PM GMT

PDB ID : 4IN7
Title : (M)L214N mutant of the Rhodobacter sphaeroides Reaction Center
Authors : Saer, R.G.; Hardjasa, A.; Murphy, M.E.P.; Beatty, J.T.
Deposited on : 2013-01-04
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 ⓘ 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

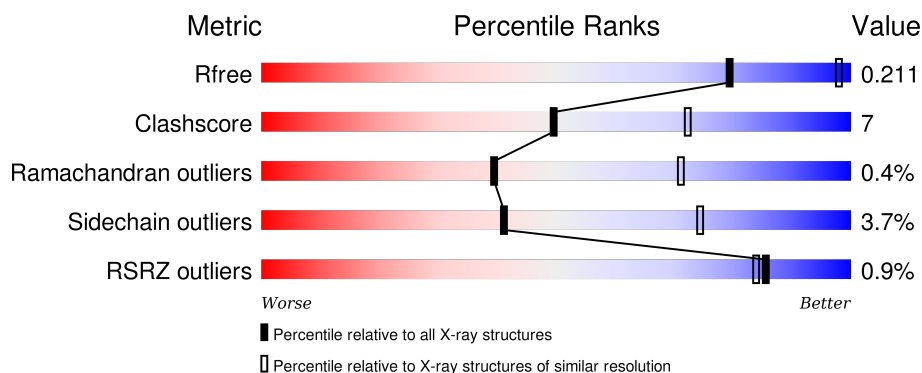
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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 $\leq 5\%$. 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	H	266	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>10%</div> </div> </div>
2	L	282	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </div> </div>
3	M	307	<div> <div></div> <div> <div></div> <div>84%</div> <div>14%</div> <div>••</div> </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	HTO	L	308	-	-	-	X
15	CDL	M	409	-	-	-	X
16	PC1	M	410	-	-	-	X
4	GOL	H	304	-	-	-	X
4	GOL	H	306	-	-	-	X
4	GOL	L	310	-	-	-	X
6	GGD	H	307	-	-	-	X
8	LDA	L	302	-	-	-	X
8	LDA	L	303	-	-	-	X
8	LDA	L	304	-	-	-	X
8	LDA	M	403	-	-	-	X
8	LDA	M	404	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7359 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	5	0
			1849	1183	320	337	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-4	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-3	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-2	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-1	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	0	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	251	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	252	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	253	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	254	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	255	MET	-	EXPRESSION TAG	UNP P0C0Y7
H	256	LEU	-	EXPRESSION TAG	UNP P0C0Y7
H	257	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	258	GLU	-	EXPRESSION TAG	UNP P0C0Y7
H	259	TYR	-	EXPRESSION TAG	UNP P0C0Y7
H	260	ALA	-	EXPRESSION TAG	UNP P0C0Y7

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	EXPRESSION TAG	UNP P0C0Y8

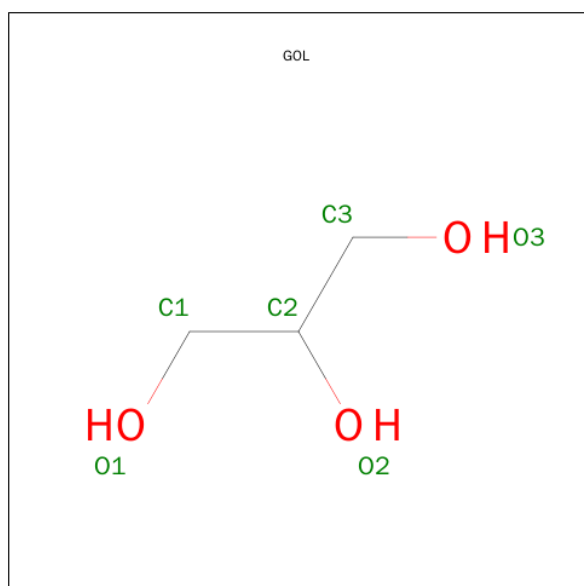
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	1	0
			2410	1605	396	399	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	EXPRESSION TAG	UNP P0C0Y9
M	214	ASN	LEU	ENGINEERED MUTATION	UNP P0C0Y9
M	303	MET	-	EXPRESSION TAG	UNP P0C0Y9
M	304	ALA	-	EXPRESSION TAG	UNP P0C0Y9
M	305	PRO	-	EXPRESSION TAG	UNP P0C0Y9
M	306	LEU	-	EXPRESSION TAG	UNP P0C0Y9

- 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	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

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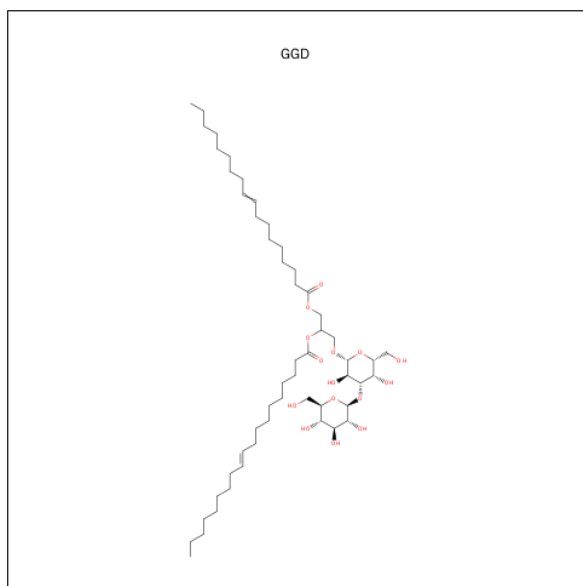
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

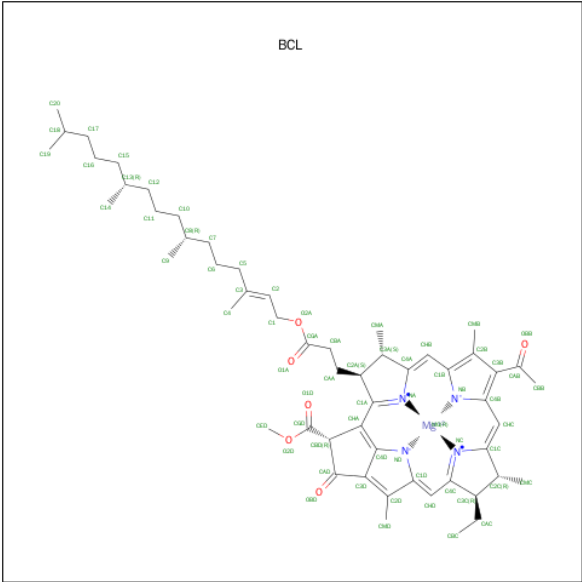
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

- Molecule 6 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: C₅₂H₉₄O₁₅).



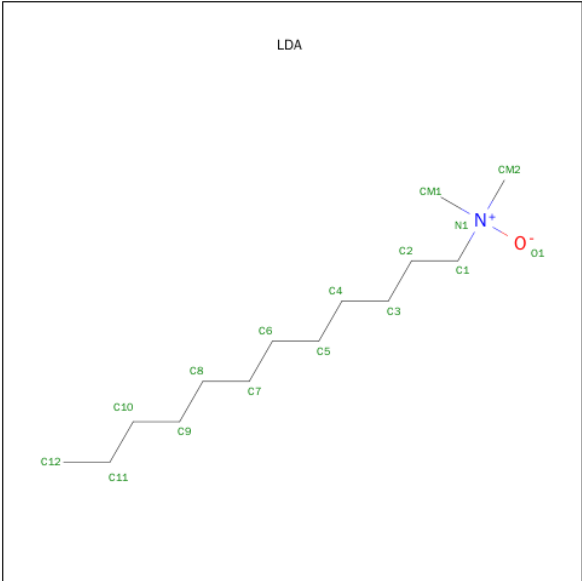
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			57	42	15		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



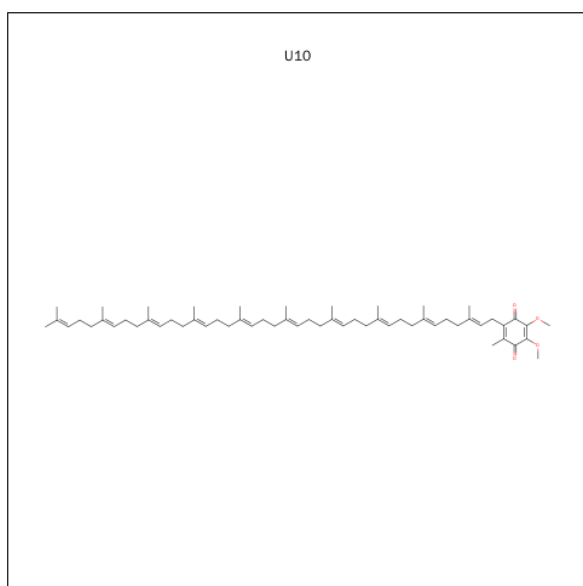
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



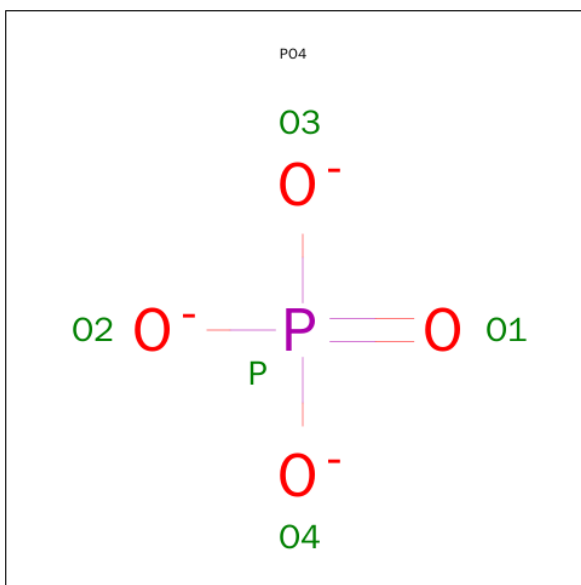
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



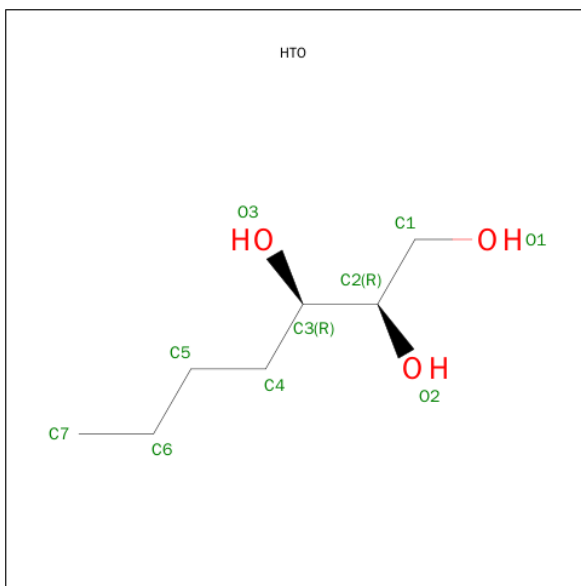
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	1
			46	38	8		
9	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 11 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

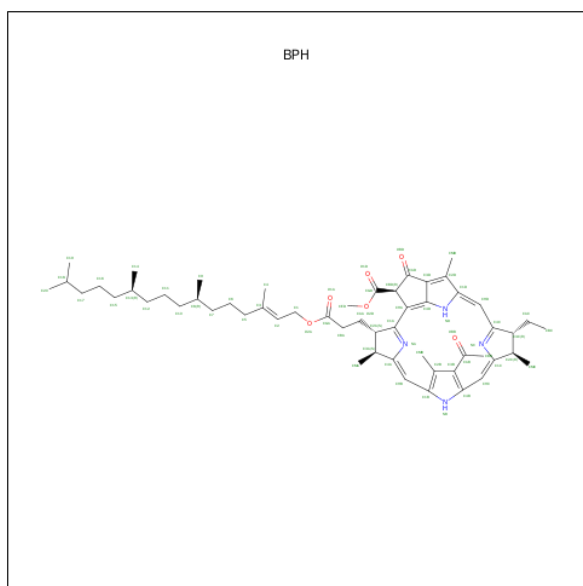


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			10	7	3		
11	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

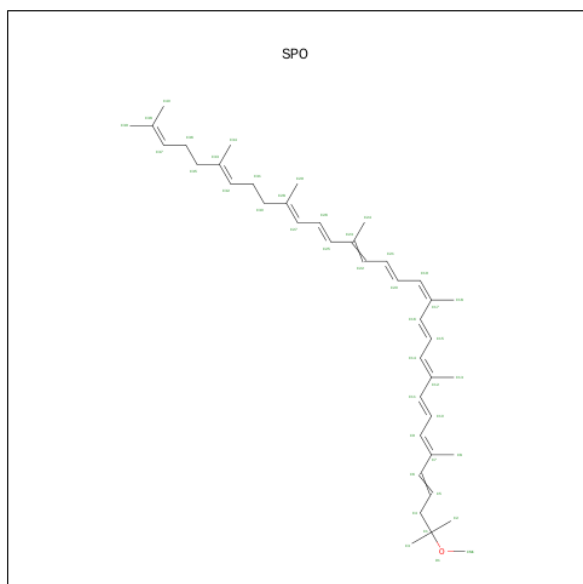
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	0
			1	1		

- Molecule 13 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



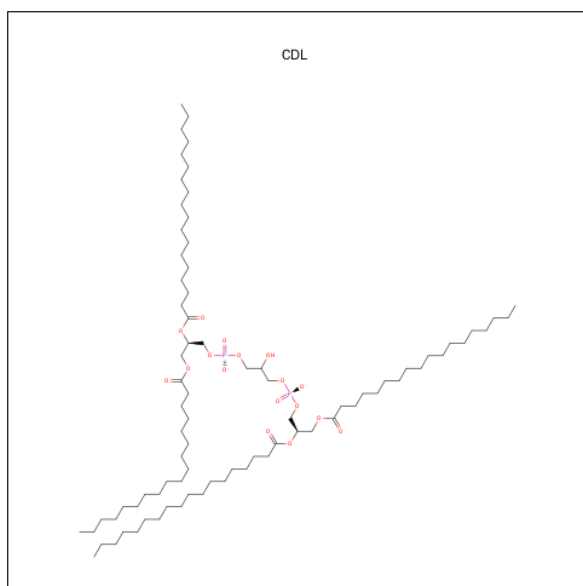
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			65	55	4	6		
13	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 14 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



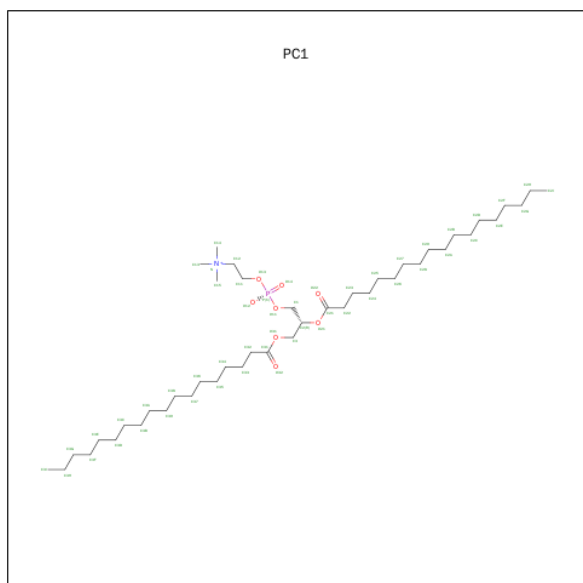
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 16 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
16	M	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

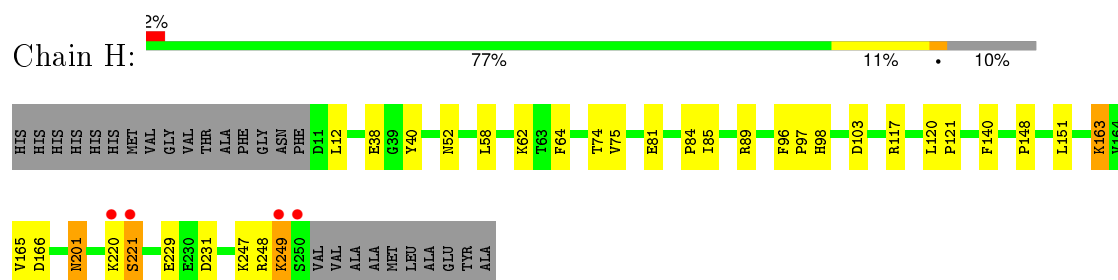
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	M	1	Total	Mg	0	0
			1	1		

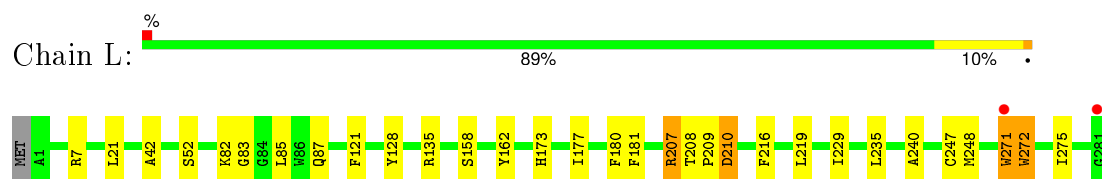
3 Residue-property plots

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

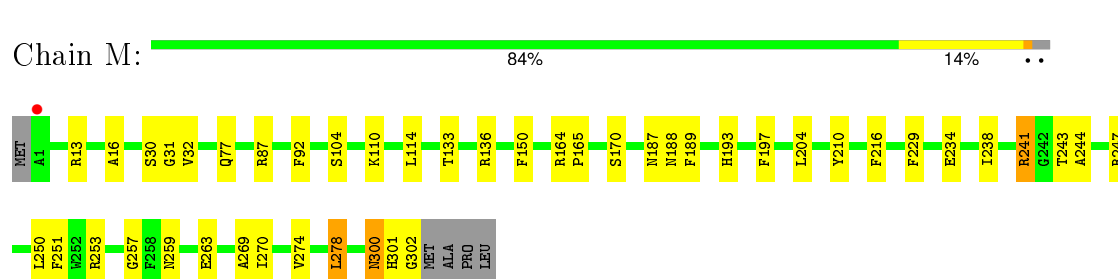
• Molecule 1: Reaction center protein H chain



• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.14Å 139.14Å 185.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.57 – 2.85 38.54 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.57-2.85) 99.9 (38.54-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.174 , 0.213 0.179 , 0.211	Depositor DCC
R_{free} test set	2474 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 48860 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CDL, BPH, K, PC1, MG, PO4, GGD, FE, SPO, U10, HTO

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	0.89	0/1929	1.05	5/2619 (0.2%)
2	L	0.85	0/2339	0.90	5/3203 (0.2%)
3	M	0.86	1/2507 (0.0%)	0.90	3/3422 (0.1%)
All	All	0.86	1/6775 (0.0%)	0.95	13/9244 (0.1%)

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
3	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	263	GLU	CD-OE1	5.51	1.31	1.25

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	210	ASP	CB-CG-OD1	7.19	124.77	118.30
2	L	207	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	H	89	ARG	NE-CZ-NH2	-6.90	116.85	120.30
3	M	241	ARG	NE-CZ-NH2	6.70	123.65	120.30
3	M	253	ARG	NE-CZ-NH1	-6.66	116.97	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	Peptide

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	1873	25	0
2	L	2239	0	2185	24	0
3	M	2410	0	2314	27	0
4	H	30	0	40	0	0
4	L	12	0	16	1	0
5	H	1	0	0	0	0
6	H	57	0	68	3	0
7	L	132	0	148	13	0
7	M	132	0	148	14	0
8	L	48	0	93	2	0
8	M	32	0	62	4	0
9	L	46	0	46	6	0
9	M	48	0	63	1	0
10	L	5	0	0	1	0
11	L	20	0	32	0	0
12	M	1	0	0	0	0
13	M	130	0	150	18	0
14	M	42	0	60	3	0
15	M	81	0	102	1	0
16	M	43	0	60	1	0
17	M	1	0	0	0	0
All	All	7359	0	7460	105	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 7.

The worst 5 of 105 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)
13:M:412:BPH:HBB3	13:M:412:BPH:HHC	1.50	0.91
13:M:406:BPH:HHC	13:M:406:BPH:HBB3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.63	0.78
1:H:248:ARG:HA	1:H:249[A]:LYS:HB2	1.68	0.75
1:H:220[B]:LYS:HE2	1:H:221:SER:OG	1.91	0.71

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	244/266 (92%)	231 (95%)	11 (4%)	2 (1%)	24	56
2	L	281/282 (100%)	265 (94%)	16 (6%)	0	100	100
3	M	301/307 (98%)	288 (96%)	11 (4%)	2 (1%)	26	59
All	All	826/855 (97%)	784 (95%)	38 (5%)	4 (0%)	39	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249[A]	LYS
1	H	249[B]	LYS
3	M	30	SER
3	M	301	HIS

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	200/214 (94%)	192 (96%)	8 (4%)	38	72
2	L	221/221 (100%)	211 (96%)	10 (4%)	34	67
3	M	237/240 (99%)	229 (97%)	8 (3%)	44	77
All	All	658/675 (98%)	632 (96%)	26 (4%)	41	72

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	210	ASP
2	L	247	CYS
3	M	259	ASN
2	L	216	PHE
2	L	235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	201	ASN
3	M	193	HIS
3	M	77	GLN
1	H	98	HIS
3	M	187	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 31 ligands modelled in this entry, 3 are 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	0.74	0	5,5,5	1.10	0
4	GOL	H	302	-	5,5,5	0.45	0	5,5,5	0.65	0
4	GOL	H	303	-	5,5,5	0.53	0	5,5,5	0.63	0
4	GOL	H	304	-	5,5,5	0.76	0	5,5,5	0.76	0
4	GOL	H	306	-	5,5,5	1.10	0	5,5,5	1.03	0
6	GGD	H	307	-	58,58,68	1.12	3 (5%)	72,72,82	1.72	14 (19%)
7	BCL	L	301	-	53,74,74	1.40	7 (13%)	57,115,115	2.45	20 (35%)
8	LDA	L	302	-	15,15,15	3.80	1 (6%)	16,17,17	1.37	1 (6%)
8	LDA	L	303	-	15,15,15	4.08	1 (6%)	16,17,17	1.72	2 (12%)
8	LDA	L	304	-	15,15,15	3.97	1 (6%)	16,17,17	0.95	1 (6%)
9	U10	L	305[A]	-	23,23,63	1.48	2 (8%)	28,31,79	1.52	7 (25%)
9	U10	L	305[B]	-	23,23,63	1.72	2 (8%)	28,31,79	1.42	5 (17%)
7	BCL	L	306	-	53,74,74	1.39	7 (13%)	57,115,115	1.48	9 (15%)
10	PO4	L	307	-	4,4,4	0.79	0	6,6,6	0.29	0
11	HTO	L	308	-	9,9,9	1.24	1 (11%)	8,10,10	1.06	0
11	HTO	L	309	-	9,9,9	1.43	1 (11%)	8,10,10	1.66	2 (25%)
4	GOL	L	310	-	5,5,5	0.42	0	5,5,5	0.50	0
4	GOL	L	311	-	5,5,5	0.32	0	5,5,5	0.34	0
7	BCL	M	401	-	53,74,74	1.60	7 (13%)	57,115,115	1.84	10 (17%)
7	BCL	M	402	-	53,74,74	1.32	7 (13%)	57,115,115	1.65	10 (17%)
8	LDA	M	403	-	15,15,15	3.95	2 (13%)	16,17,17	1.99	2 (12%)
8	LDA	M	404	-	15,15,15	3.81	1 (6%)	16,17,17	1.21	3 (18%)
13	BPH	M	406	-	64,70,70	1.92	14 (21%)	73,101,101	1.96	18 (24%)
9	U10	M	407	-	48,48,63	1.30	5 (10%)	58,61,79	2.45	19 (32%)
14	SPO	M	408	-	40,41,41	0.79	1 (2%)	45,50,50	1.93	10 (22%)
15	CDL	M	409	-	79,79,99	1.47	5 (6%)	80,90,111	1.45	8 (10%)
16	PC1	M	410	-	42,42,53	1.47	4 (9%)	46,50,61	1.61	5 (10%)
13	BPH	M	412	-	64,70,70	1.93	15 (23%)	73,101,101	2.47	19 (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	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
4	GOL	H	306	-	-	0/4/4/4	0/0/0/0
6	GGD	H	307	-	-	0/47/87/97	0/2/2/2
7	BCL	L	301	-	-	0/37/137/137	0/0/9/9
8	LDA	L	302	-	-	0/13/13/13	0/0/0/0
8	LDA	L	303	-	-	0/13/13/13	0/0/0/0
8	LDA	L	304	-	-	0/13/13/13	0/0/0/0
9	U10	L	305[A]	-	-	0/15/39/87	0/1/1/1
9	U10	L	305[B]	-	-	0/15/39/87	0/1/1/1
7	BCL	L	306	-	-	0/37/137/137	0/0/9/9
10	PO4	L	307	-	-	0/0/0/0	0/0/0/0
11	HTO	L	308	-	-	0/10/10/10	0/0/0/0
11	HTO	L	309	-	-	0/10/10/10	0/0/0/0
4	GOL	L	310	-	-	0/4/4/4	0/0/0/0
4	GOL	L	311	-	-	0/4/4/4	0/0/0/0
7	BCL	M	401	-	-	0/37/137/137	0/0/9/9
7	BCL	M	402	-	-	0/37/137/137	0/0/9/9
8	LDA	M	403	-	-	0/13/13/13	0/0/0/0
8	LDA	M	404	-	-	0/13/13/13	0/0/0/0
13	BPH	M	406	-	-	0/54/105/105	0/1/6/6
9	U10	M	407	-	-	0/45/69/87	0/1/1/1
14	SPO	M	408	-	-	0/47/47/47	0/0/0/0
15	CDL	M	409	-	-	0/88/88/110	0/0/0/0
16	PC1	M	410	-	-	0/46/46/57	0/0/0/0
13	BPH	M	412	-	-	0/54/105/105	0/1/6/6

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	303	LDA	O1-N1	-15.55	1.24	1.39
8	L	304	LDA	O1-N1	-15.26	1.25	1.39
8	M	403	LDA	O1-N1	-14.77	1.25	1.39
8	M	404	LDA	O1-N1	-14.61	1.25	1.39
8	L	302	LDA	O1-N1	-14.42	1.25	1.39

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	408	SPO	C4-C5-C6	-7.08	114.60	124.67
9	M	407	U10	C31-C29-C28	-6.54	108.64	121.05
8	M	403	LDA	O1-N1-CM2	-6.54	100.31	109.05
13	M	412	BPH	CED-O2D-CGD	-6.13	101.60	115.99
8	L	303	LDA	O1-N1-CM2	-5.92	101.14	109.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	307	GGD	3	0
7	L	301	BCL	7	0
8	L	304	LDA	2	0
9	L	305[B]	U10	6	0
7	L	306	BCL	7	0
10	L	307	PO4	1	0
4	L	311	GOL	1	0
7	M	401	BCL	7	0
7	M	402	BCL	9	0
8	M	403	LDA	2	0
8	M	404	LDA	2	0
13	M	406	BPH	6	0
9	M	407	U10	1	0
14	M	408	SPO	3	0
15	M	409	CDL	1	0
16	M	410	PC1	1	0
13	M	412	BPH	12	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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	240/266 (90%)	-0.47	4 (1%)	73 70	33, 43, 61, 133	3 (1%)
2	L	281/282 (99%)	-0.63	2 (0%)	89 88	30, 41, 64, 89	0
3	M	302/307 (98%)	-0.46	1 (0%)	94 93	31, 45, 66, 99	6 (1%)
All	All	823/855 (96%)	-0.52	7 (0%)	85 84	30, 43, 64, 133	9 (1%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	7.3
1	H	249[A]	LYS	3.3
3	M	1	ALA	3.2
2	L	281	GLY	2.5
2	L	271[A]	TRP	2.4

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, 95th 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
8	LDA	L	303	16/16	0.57	0.54	22.43	80,90,108,114	0
11	HTO	L	308	10/10	0.84	0.50	16.51	66,87,102,105	0
8	LDA	L	302	16/16	0.67	0.57	15.85	47,125,153,155	0
4	GOL	L	310	6/6	0.87	0.46	8.22	73,81,85,86	0
16	PC1	M	410	43/54	0.47	0.45	6.55	61,99,145,170	0
15	CDL	M	409	81/100	0.85	0.40	6.50	53,96,139,153	0
4	GOL	H	306	6/6	0.78	0.36	5.83	69,76,89,90	0
8	LDA	L	304	16/16	0.58	0.40	5.58	71,98,123,128	0
8	LDA	M	404	16/16	0.91	0.33	5.35	59,69,92,96	0
6	GGD	H	307	57/67	0.75	0.41	4.32	51,108,185,203	0
4	GOL	H	304	6/6	0.92	0.32	3.71	40,52,63,71	0
8	LDA	M	403	16/16	0.92	0.20	2.08	52,68,77,78	0
9	U10	L	305[A]	23/63	0.92	0.26	1.83	33,37,65,71	23
9	U10	L	305[B]	23/63	0.92	0.26	1.49	35,50,60,62	23
9	U10	M	407	48/63	0.94	0.24	1.46	33,46,91,110	0
14	SPO	M	408	42/42	0.94	0.21	1.43	33,47,80,92	0
13	BPH	M	406	65/65	0.93	0.23	1.27	35,47,119,134	0
7	BCL	M	402	66/66	0.98	0.20	1.16	33,40,51,75	0
7	BCL	M	401	66/66	0.97	0.21	1.08	28,38,95,105	0
7	BCL	L	306	66/66	0.97	0.15	0.55	28,39,49,65	0
13	BPH	M	412	65/65	0.98	0.15	0.18	30,39,48,57	0
5	K	H	305	1/1	0.96	0.12	-0.21	50,50,50,50	0
7	BCL	L	301	66/66	0.97	0.13	-0.45	26,34,56,61	0
10	PO4	L	307	5/5	0.96	0.11	-0.75	60,62,66,67	0
12	FE	M	405	1/1	0.99	0.16	-0.80	36,36,36,36	0
4	GOL	H	303	6/6	0.76	0.42	-	85,89,92,95	0
11	HTO	L	309	10/10	0.70	0.86	-	72,96,120,121	0
4	GOL	H	301	6/6	0.90	0.39	-	59,65,69,80	0
17	MG	M	411	1/1	0.96	0.15	-	39,39,39,39	0
4	GOL	H	302	6/6	0.85	0.34	-	81,82,85,90	0
4	GOL	L	311	6/6	0.83	0.33	-	83,88,91,94	0

6.5 Other polymers

There are no such residues in this entry.